

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
 Data File : BP018788.D
 Acq On : 13 Dec 2023 03:03
 Operator : MA/JU
 Sample : 05646-11
 Misc :
 ALS Vial : 67 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AY7

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018788.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.687	99	102	110	rBV	79432	127794	0.26%	0.079%
2	5.152	343	351	364	rVB	13088161	21533247	44.16%	13.321%
3	6.817	628	634	642	rBV4	19221	53223	0.11%	0.033%
4	7.005	656	666	678	rVB2	368800	728986	1.50%	0.451%
5	7.175	688	695	709	rVB	307965	476738	0.98%	0.295%
6	7.369	720	728	740	rVB	389600	646647	1.33%	0.400%
7	7.722	781	788	797	rVB	1239097	1979481	4.06%	1.225%
8	7.840	800	808	810	rBV	616526	1034389	2.12%	0.640%
9	7.875	810	814	823	rVB	2216499	3402623	6.98%	2.105%
10	8.187	862	867	872	rVB	50478	75041	0.15%	0.046%
11	8.546	921	928	935	rBV	454958	728576	1.49%	0.451%
12	8.663	942	948	955	rVB	259205	408274	0.84%	0.253%
13	8.999	998	1005	1013	rVB	356351	575295	1.18%	0.356%
14	9.558	1092	1100	1104	rBV	29805	50250	0.10%	0.031%
15	9.605	1104	1108	1116	rVB	35510	73407	0.15%	0.045%
16	9.716	1119	1127	1133	rBV	283549	461176	0.95%	0.285%
17	9.775	1133	1137	1145	rVB	39330	69274	0.14%	0.043%
18	9.887	1145	1156	1164	rBV	82915	185355	0.38%	0.115%
19	10.081	1183	1189	1197	rVB	31019	53838	0.11%	0.033%
20	10.252	1211	1218	1228	rBV	479221	808584	1.66%	0.500%
21	10.528	1257	1265	1272	rBV	21411	53766	0.11%	0.033%
22	10.634	1274	1283	1290	rVV	766665	1300732	2.67%	0.805%
23	10.775	1299	1307	1318	rBV	179611	341359	0.70%	0.211%
24	11.175	1369	1375	1384	rBV3	25703	55643	0.11%	0.034%
25	12.804	1646	1652	1660	rBV	31167	61563	0.13%	0.038%
26	13.393	1744	1752	1758	rBV2	81347	143765	0.29%	0.089%
27	13.881	1829	1835	1843	rBV	854474	1160447	2.38%	0.718%
28	14.157	1874	1882	1894	rBV	966596	1393892	2.86%	0.862%
29	14.463	1928	1934	1942	rBV	1175152	1803239	3.70%	1.116%
30	14.669	1962	1969	1986	rBV	252084	445244	0.91%	0.275%
31	14.822	1990	1995	2001	rVV	34938	49857	0.10%	0.031%
32	15.457	2096	2103	2109	rBV	1270781	1827992	3.75%	1.131%
33	15.575	2117	2123	2133	rVV	249321	357747	0.73%	0.221%
34	17.216	2395	2402	2412	rBV	1636773	2343948	4.81%	1.450%
35	17.310	2412	2418	2428	rVV2	1346665	1935917	3.97%	1.198%
36	18.104	2548	2553	2563	rBV	232762	345949	0.71%	0.214%

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37	18.663	2644	2648	2654	rVB	75806	105905	0.22%	0.066%
38	18.881	2681	2685	2688	rBV	66931	80158	0.16%	0.050%
39	19.004	2702	2706	2710	rVV	44127	52623	0.11%	0.033%
40	19.128	2719	2727	2736	rBV7	85048	262979	0.54%	0.163%
41	19.339	2759	2763	2770	rBV2	110434	153197	0.31%	0.095%
42	19.551	2793	2799	2806	rBV	1921718	2674548	5.49%	1.655%
43	19.881	2852	2855	2859	rBV	64683	71187	0.15%	0.044%
44	20.081	2886	2889	2894	rVB	225436	241319	0.49%	0.149%
45	20.633	2976	2983	2993	rVB8	123533	286718	0.59%	0.177%
46	20.728	2994	2999	3003	rBV	1637177	2096600	4.30%	1.297%
47	20.763	3003	3005	3008	rVV2	175207	176376	0.36%	0.109%
48	20.798	3008	3011	3015	rVB	312219	366611	0.75%	0.227%
49	20.916	3025	3031	3035	rBV	6610708	7944123	16.29%	4.914%
50	20.957	3035	3038	3044	rVB2	365881	508318	1.04%	0.314%
51	21.022	3044	3049	3051	rBV	1148092	1568918	3.22%	0.971%
52	21.051	3051	3054	3060	rVB	3682993	4460748	9.15%	2.759%
53	21.157	3069	3072	3078	rBV3	140459	201679	0.41%	0.125%
54	21.263	3083	3090	3093	rVV2	893098	1353515	2.78%	0.837%
55	21.304	3093	3097	3102	rVB	2664423	3350467	6.87%	2.073%
56	21.904	3195	3199	3201	rBV	552317	687470	1.41%	0.425%
57	21.933	3201	3204	3213	rVB2	999331	1857948	3.81%	1.149%
58	22.539	3303	3307	3315	rVB3	336569	540949	1.11%	0.335%
59	22.645	3321	3325	3329	rVB	196166	273174	0.56%	0.169%
60	22.945	3370	3376	3381	rBV	1211235	1879765	3.86%	1.163%
61	23.004	3381	3386	3396	rVV	850622	1943837	3.99%	1.202%
62	23.510	3466	3472	3478	rBV2	1476094	2708404	5.55%	1.675%
63	23.663	3491	3498	3505	rBV	1635595	3188784	6.54%	1.973%
64	24.274	3597	3602	3611	rVB	446898	969057	1.99%	0.599%
65	24.386	3615	3621	3633	rBV	537843	1683638	3.45%	1.042%
66	25.057	3729	3735	3751	rVB	1157971	2942960	6.04%	1.821%
67	25.621	3823	3831	3841	rVB3	722444	1993341	4.09%	1.233%
68	25.963	3883	3889	3898	rVB	408639	1030906	2.11%	0.638%
69	26.145	3915	3920	3931	rVB2	950786	2602291	5.34%	1.610%
70	27.221	4093	4103	4123	rVB4	1482583	5332088	10.94%	3.299%
71	27.451	4135	4142	4153	rVB2	733444	2271309	4.66%	1.405%
72	28.074	4230	4248	4264	rVB2	11160483	48757443	100.00%	30.162%
73	28.457	4300	4313	4330	rBV5	1682780	7938677	16.28%	4.911%

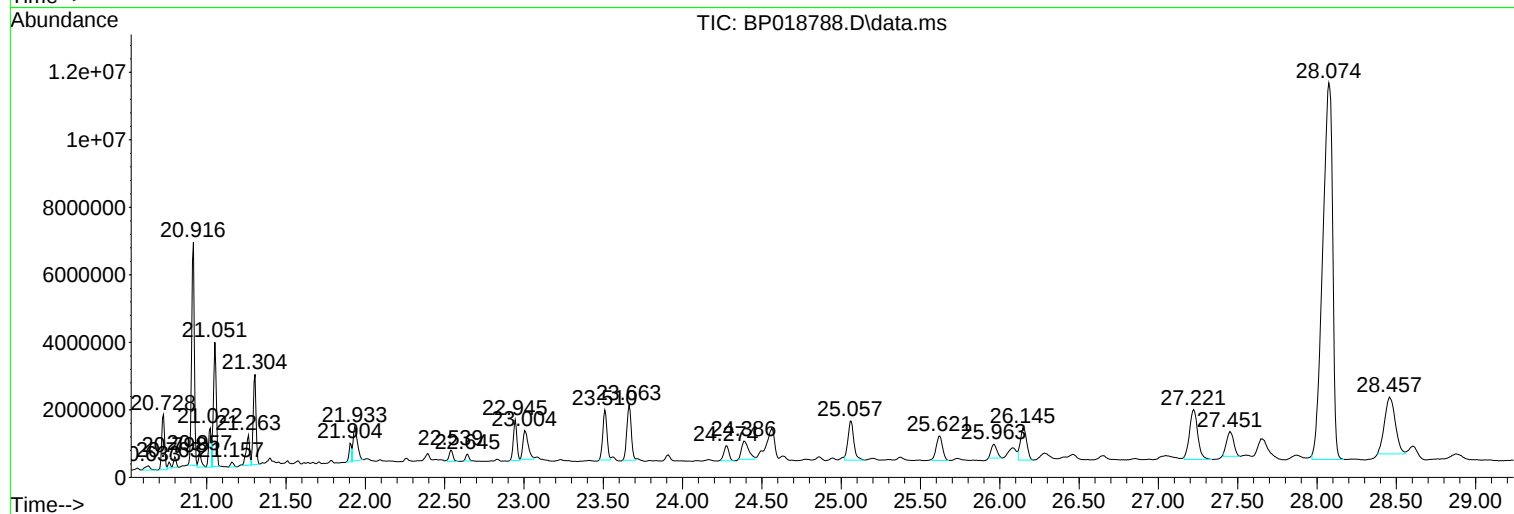
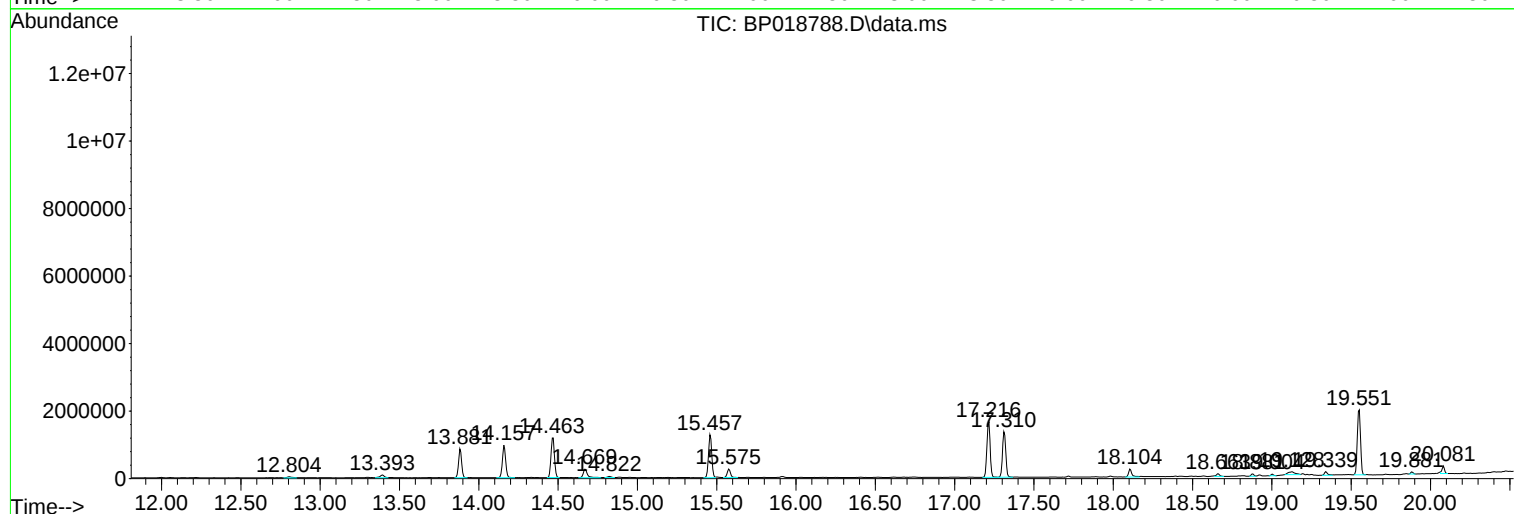
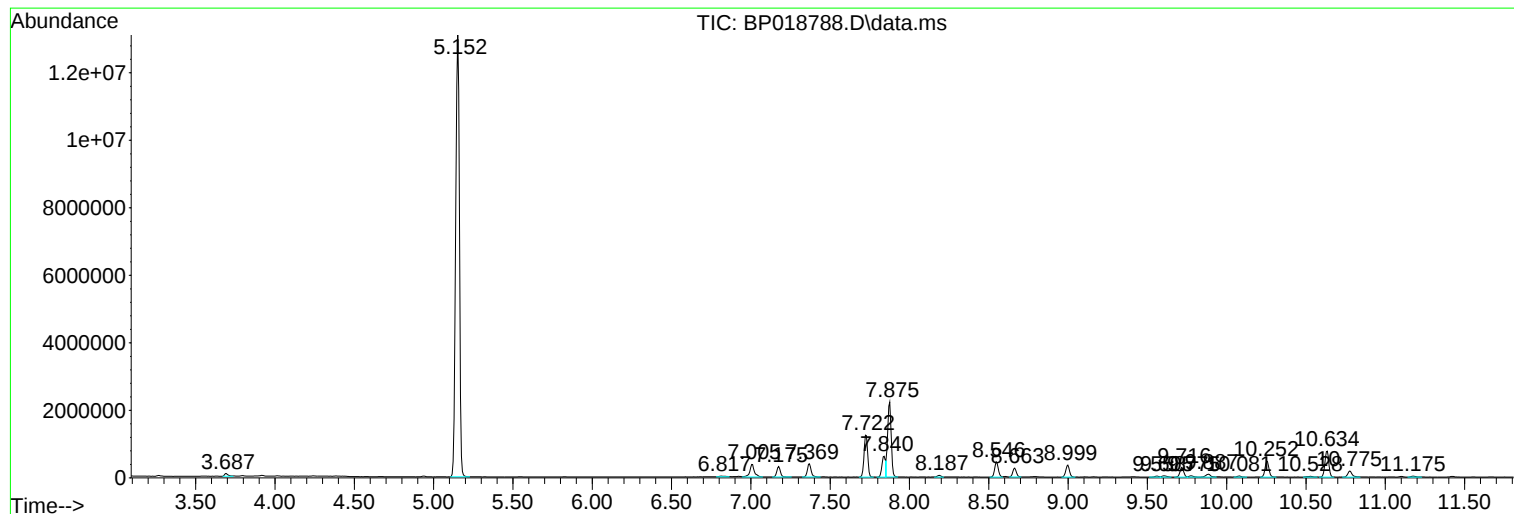
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P



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Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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C0AY7

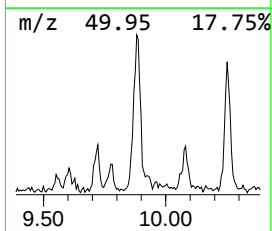
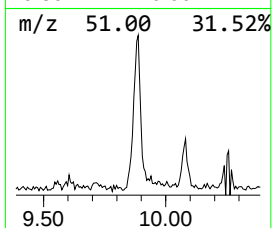
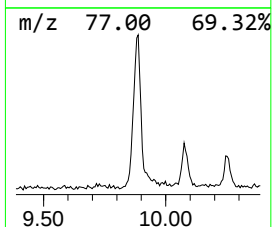
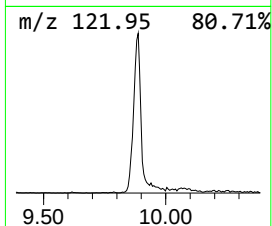
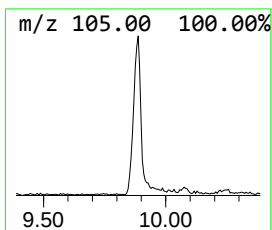
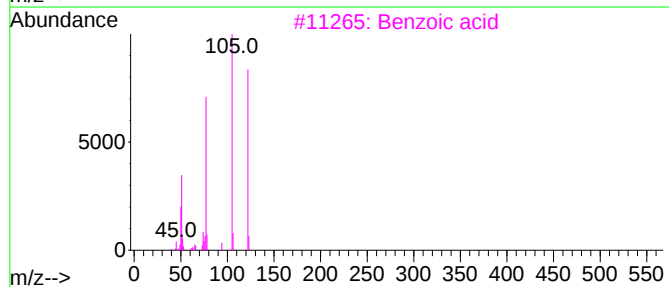
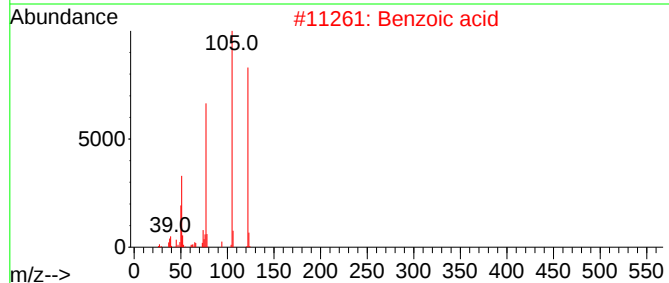
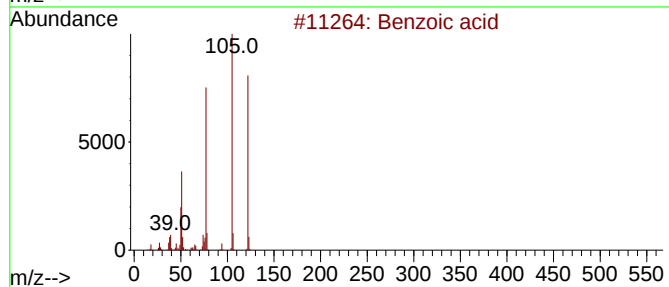
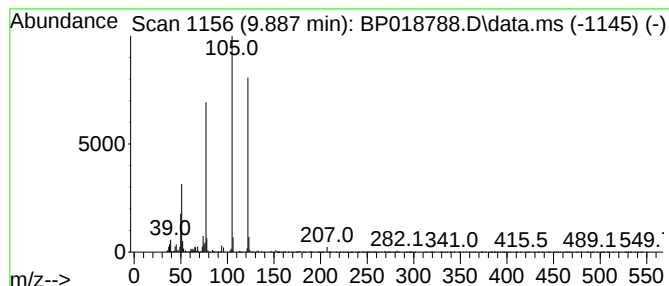
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzoic acid Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.887	2.85 ng/ul	185355	Naphthalene-d8	10.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	96
2			Benzoic acid	122	C7H6O2	000065-85-0	96
3			Benzoic acid	122	C7H6O2	000065-85-0	96
4			Benzoic acid	122	C7H6O2	000065-85-0	94
5			Heptanediamide, N,N'-di-benzoyloxy-	398	C21H22N2O6	1000253-26-4	91



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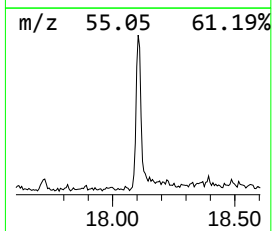
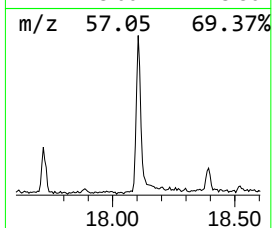
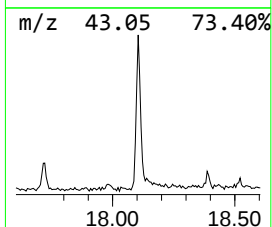
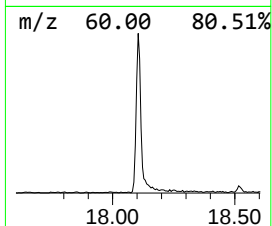
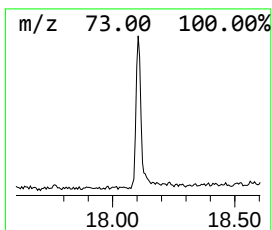
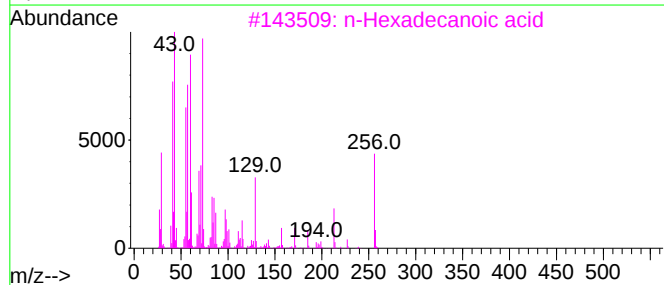
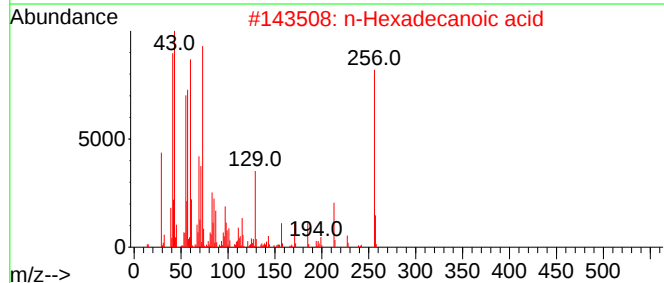
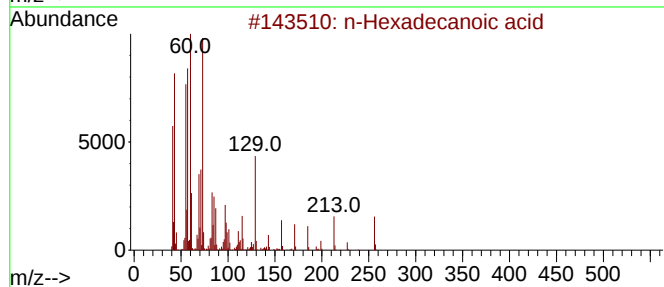
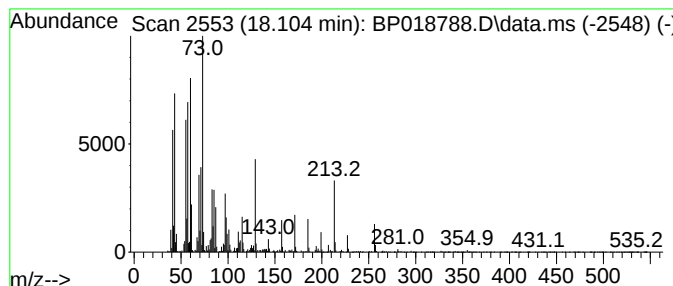
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.104	2.95 ng/ul	345949	Phenanthrene-d10	17.216	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5	Octadecanoic acid	284	C18H36O2	000057-11-4	90



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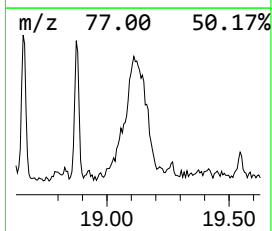
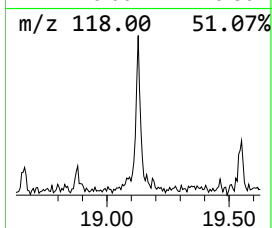
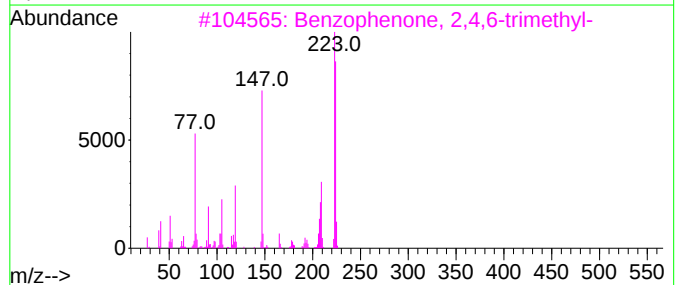
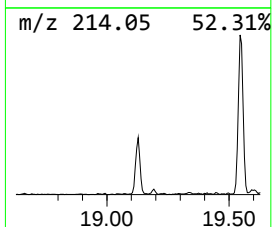
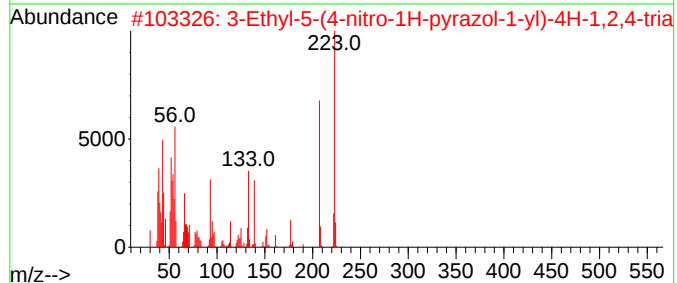
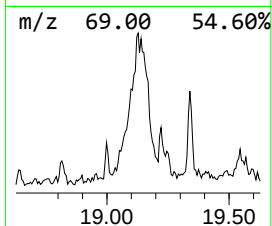
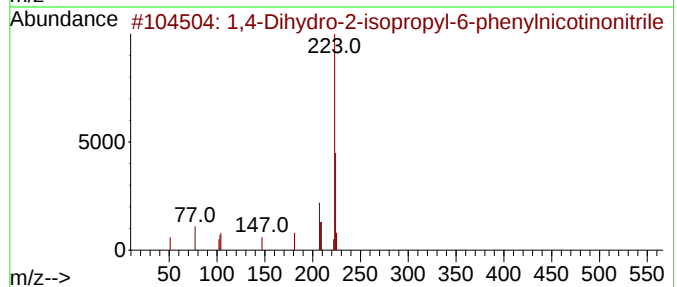
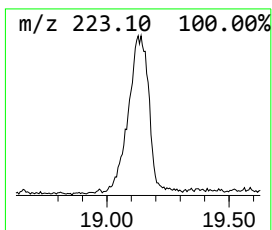
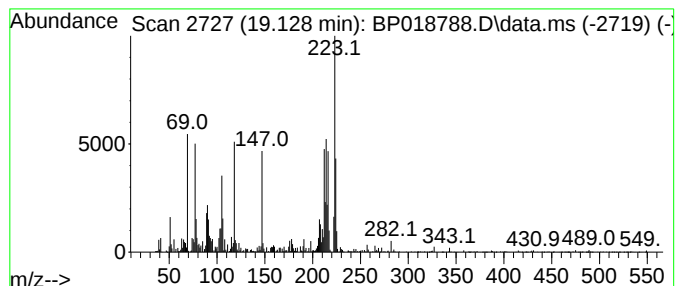
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-01 Concentration Rank 25

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.128	2.24 ng/ul	262979	Phenanthrene-d10	17.216	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dihydro-2-isopropyl-6-phenyl...	224	C15H16N2	070231-37-7	25
2	3-Ethyl-5-(4-nitro-1H-pyrazol-1-...	223	C7H9N7O2	1000387-05-7	25
3	Benzophenone, 2,4,6-trimethyl-	224	C16H16O	000954-16-5	18
4	1H-Pyrrolo[3,2-H]quinoline, 2,3,...	224	C15H16N2	1000311-11-7	18
5	Dibenzoylmethane	224	C15H12O2	000120-46-7	15



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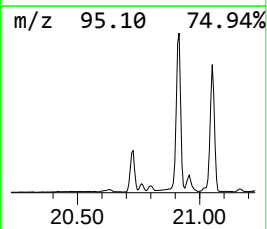
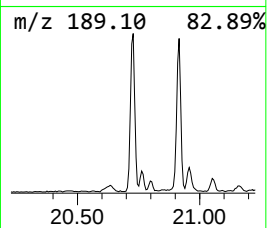
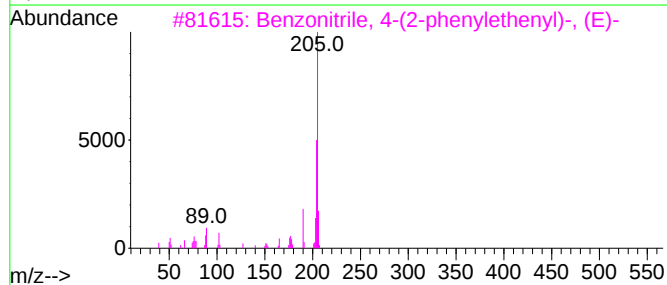
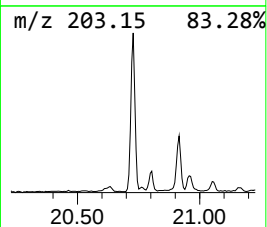
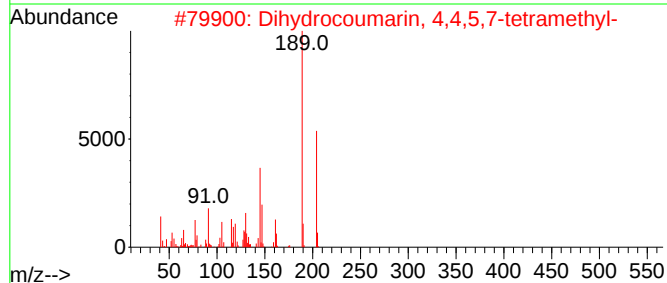
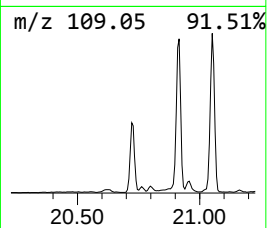
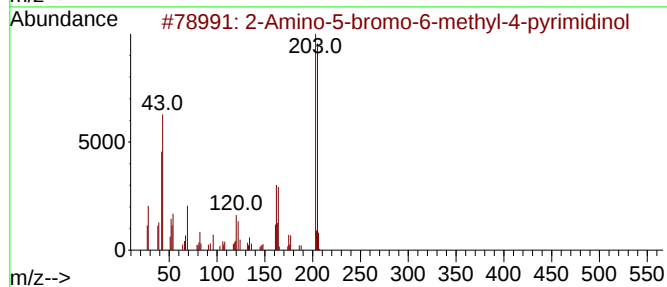
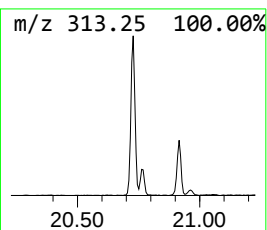
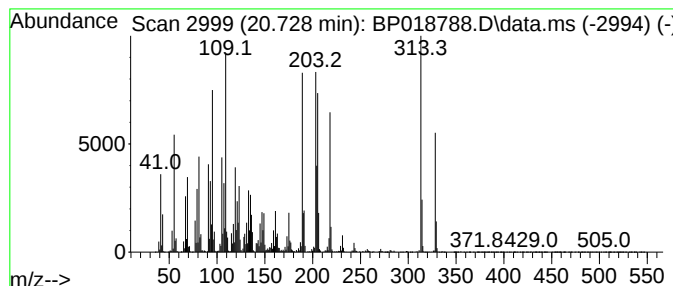
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-02 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.728	12.52 ng/ul	2096600	Chrysene-d12	21.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-5-bromo-6-methyl-4-pyrim...	203	C5H6BrN3O	006307-35-3	25
2	Dihydrocoumarin, 4,4,5,7-tetrame...	204	C13H16O2	040662-14-4	15
3	Benzonitrile, 4-(2-phenylethenyl)...	205	C15H11N	013041-79-7	15
4	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	15
5	Indolizine, 1-acetyl-2-methyl-6-...	218	C11H10N2O3	100071-33-1	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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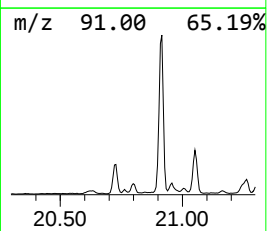
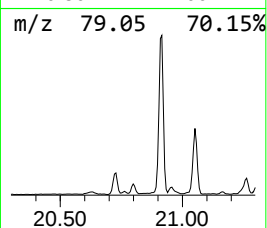
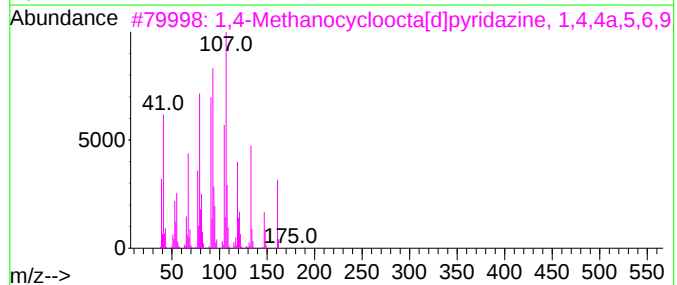
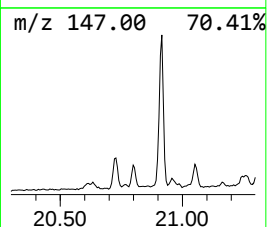
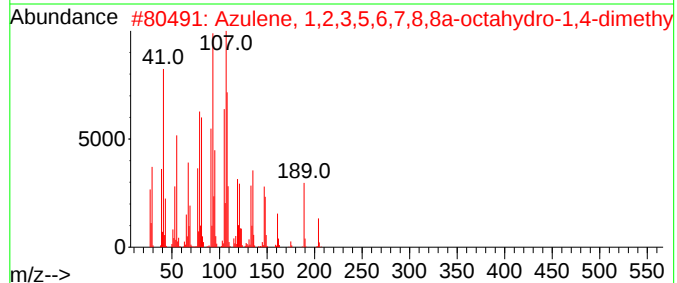
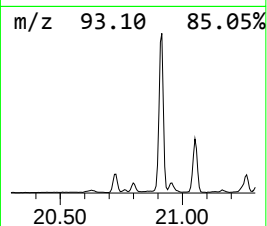
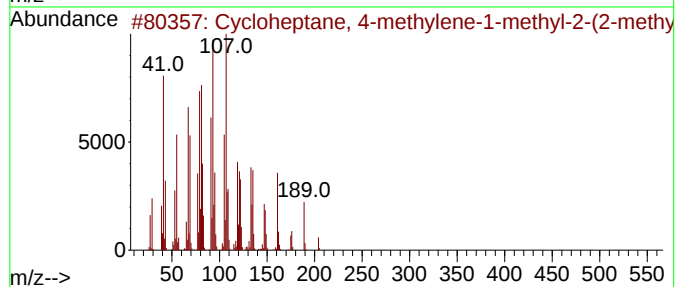
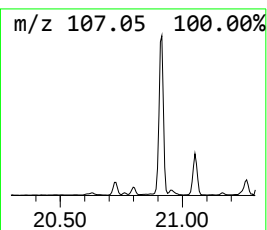
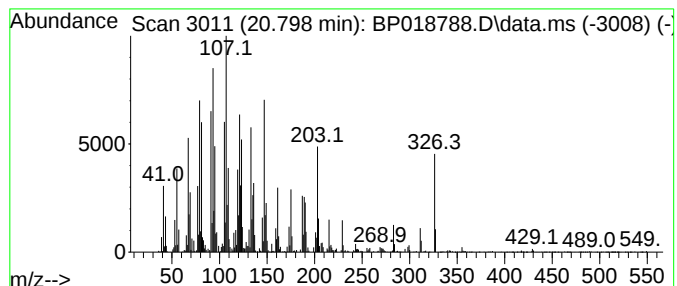
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cycloheptane, 4-methylene-1... Concentration Rank 26

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.798	2.19 ng/ul	366611	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptane, 4-methylene-1-meth...	204	C15H24	1010159-38-5	55
2			Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	50
3			1,4-Methanocycloocta[d]pyridazin...	204	C13H20N2	1000221-85-9	46
4			1-Cycloheptene, 1,4-dimethyl-3-(...	204	C15H24	1000159-38-6	38
5			Bis(2-methyl-3-vinylcyclopent-2-...	230	C16H22O	1000142-16-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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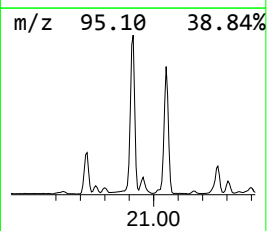
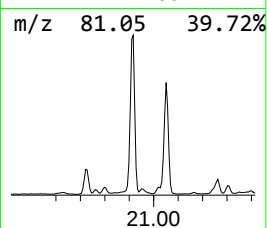
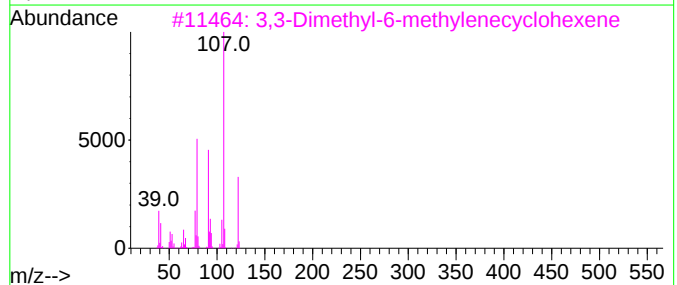
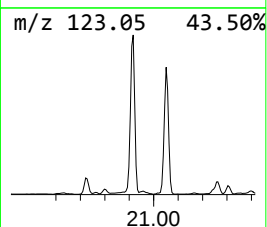
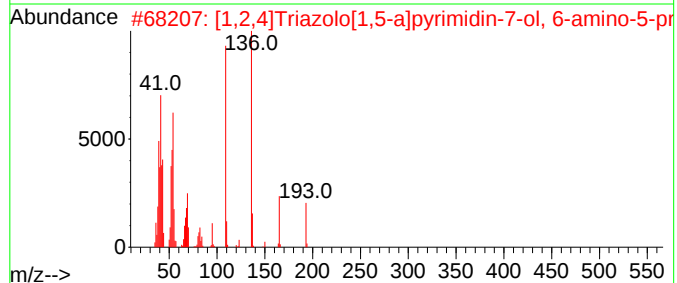
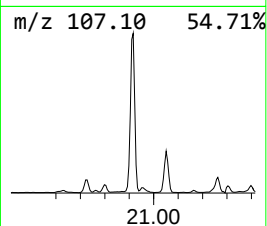
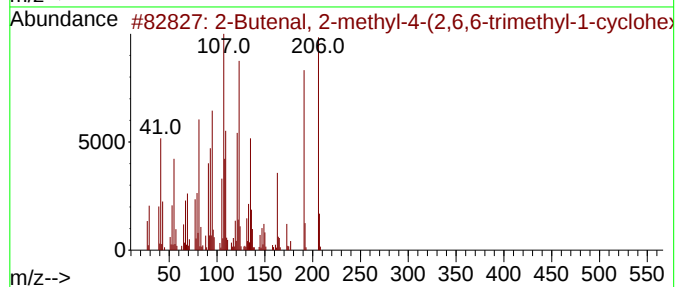
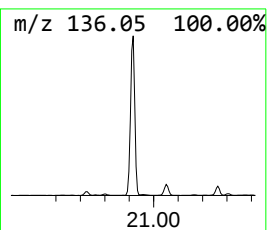
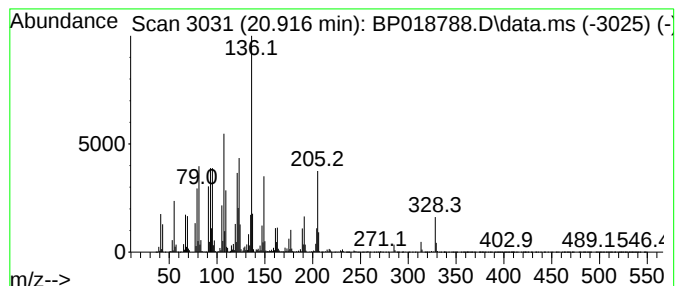
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2-Butenal, 2-methyl-4-(2,6,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.916	47.42 ng/ul	7944120	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	64
2			[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000362-66-7	35
3			3,3-Dimethyl-6-methylenecyclohexene	122	C9H14	020185-16-4	25
4			3-Cyclopentylpropionamide, N-phe...	231	C15H21NO	1000340-38-2	25
5			4-Fluoro-7-azaindole	136	C7H5FN2	640735-23-5	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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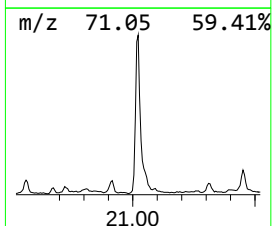
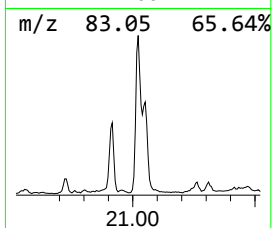
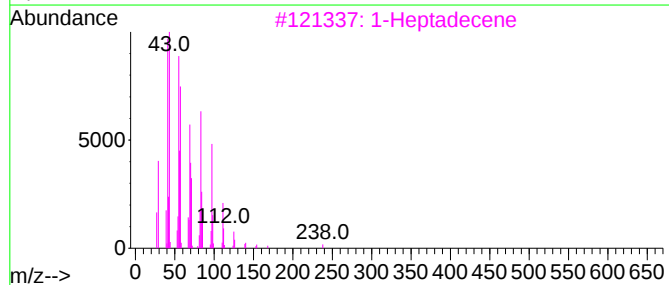
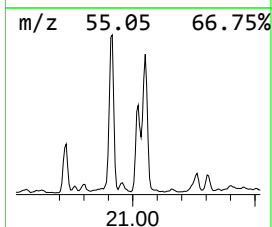
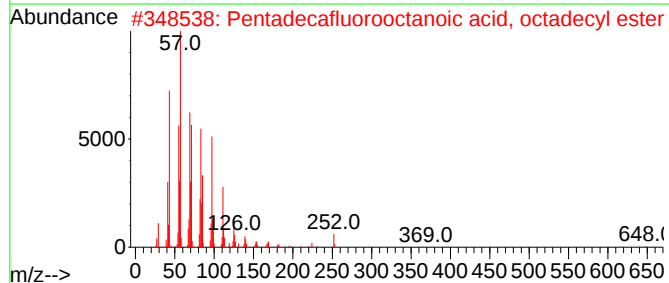
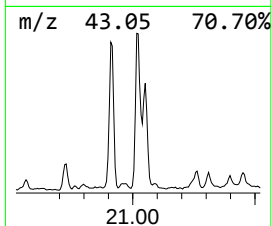
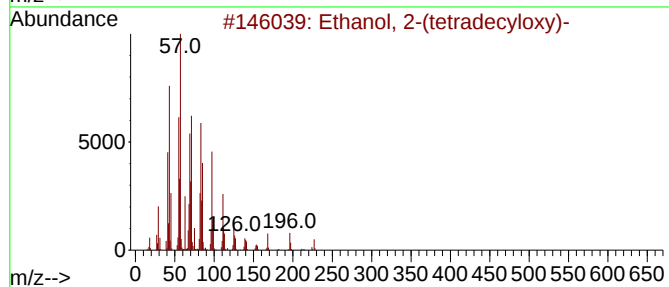
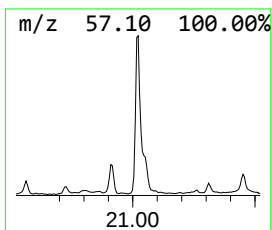
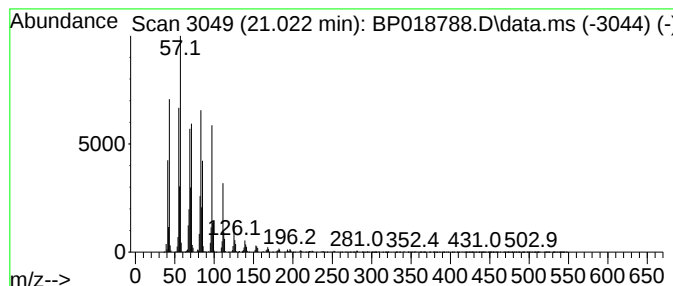
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Ethanol, 2-(tetradecyloxy)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	9.37 ng/ul	1568920	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			1-Heptadecene	238	C17H34	006765-39-5	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
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Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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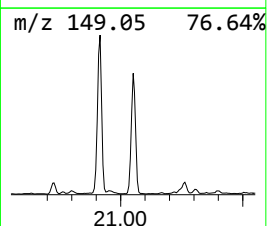
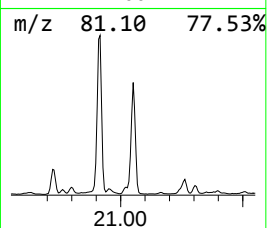
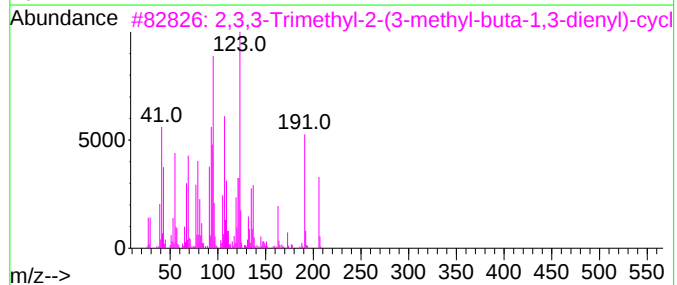
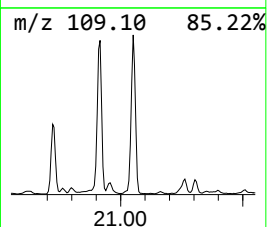
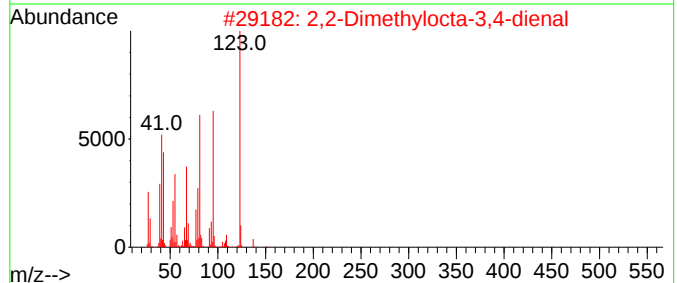
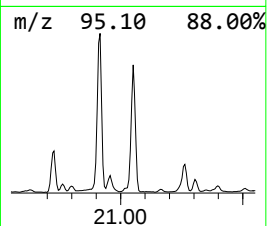
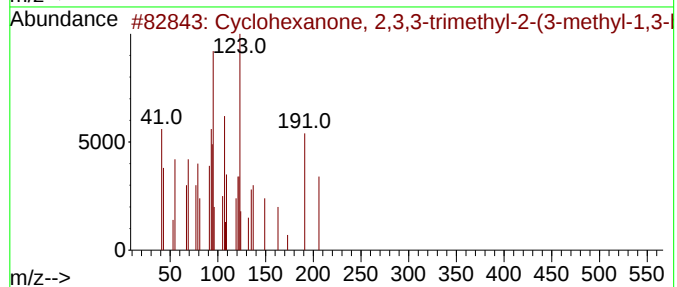
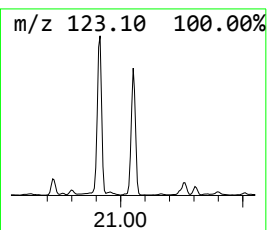
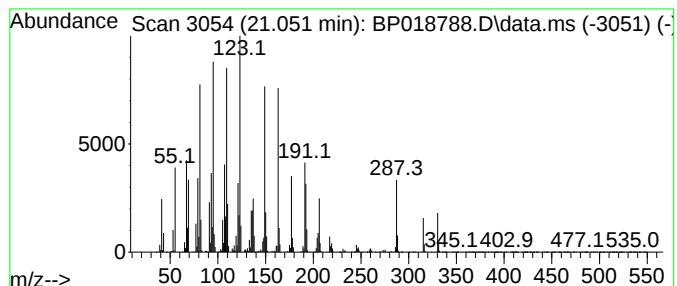
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Cyclohexanone, 2,3,3-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	26.63 ng/ul	4460750	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	53
2			2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	35
3			2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	30
4			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	25
5			2H-Cycloprop[c]indene-2,3(3ah)-d...	206	C13H18O2	096678-99-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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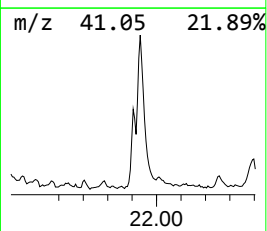
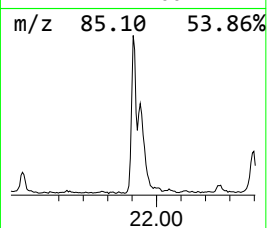
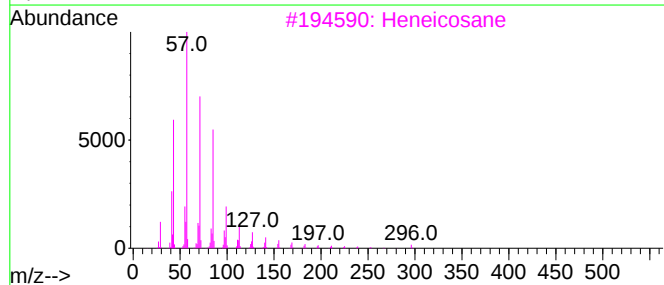
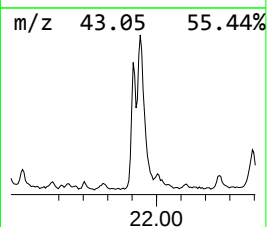
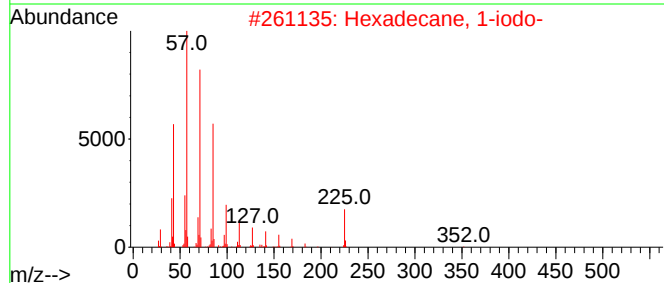
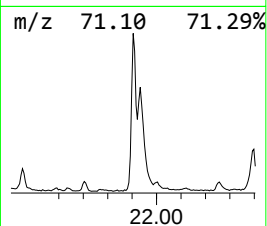
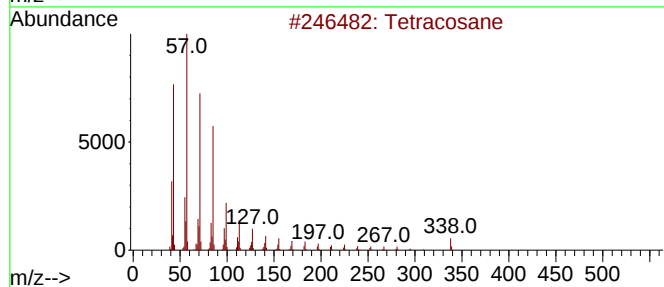
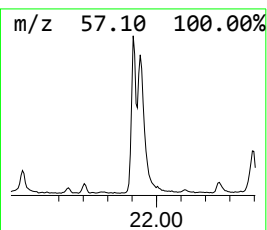
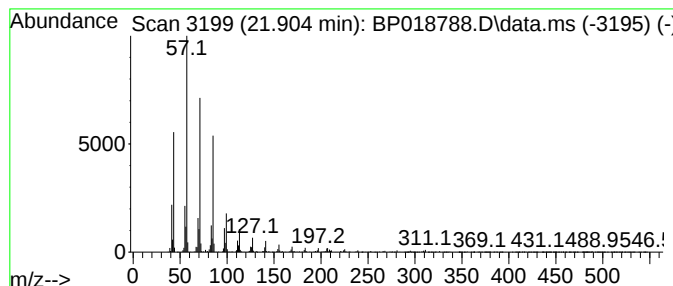
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 (DEL) Alkane: Straight-Chai... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.904	4.10 ng/ul	687470	Chrysene-d12	21.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	97
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
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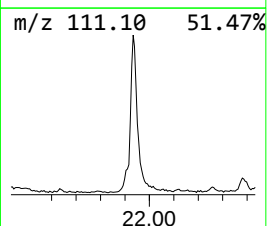
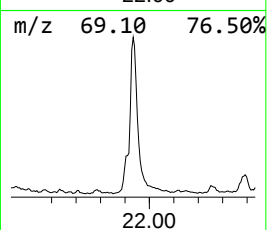
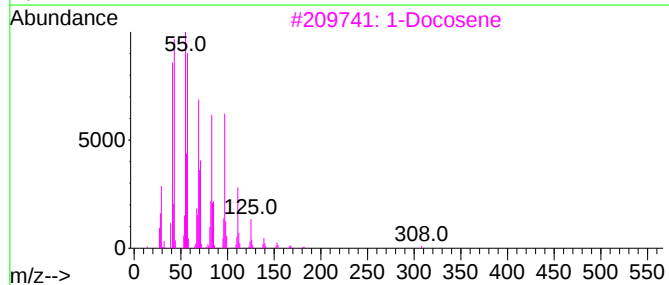
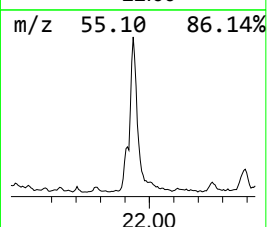
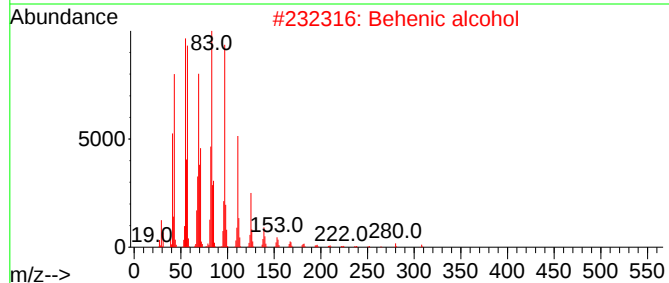
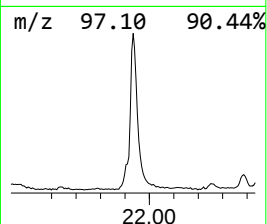
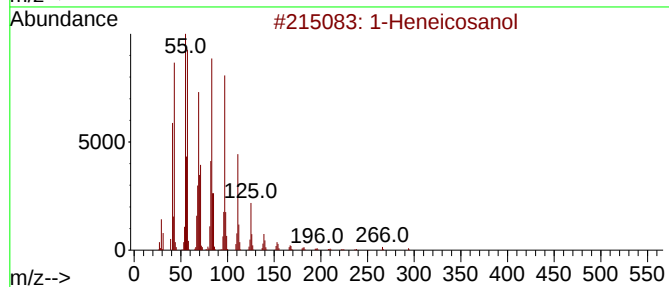
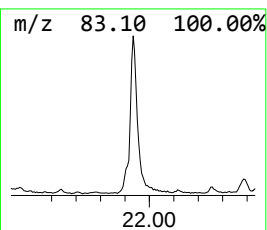
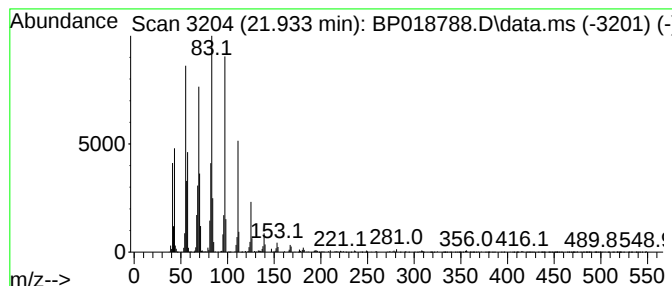
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1-Heneicosanol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.933	11.09 ng/ul	1857950	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	91
2			Behenic alcohol	326	C22H46O	000661-19-8	90
3			1-Docosene	308	C22H44	001599-67-3	83
4			1-Octadecanol	270	C18H38O	000112-92-5	58
5			1-Hexadecanol	242	C16H34O	036653-82-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

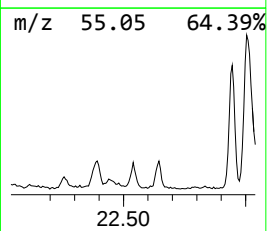
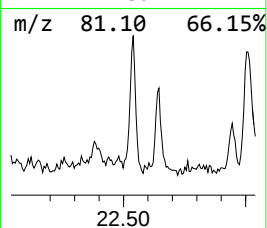
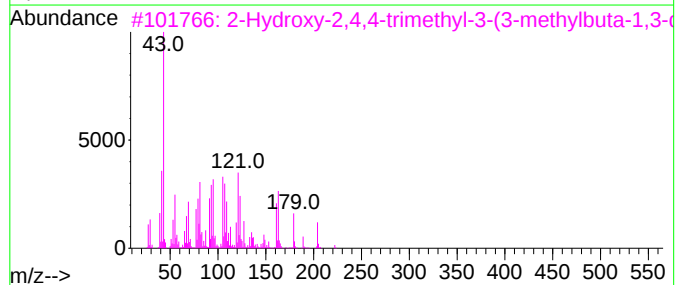
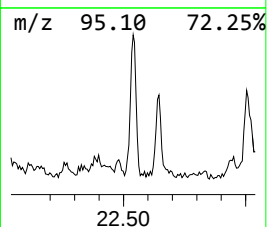
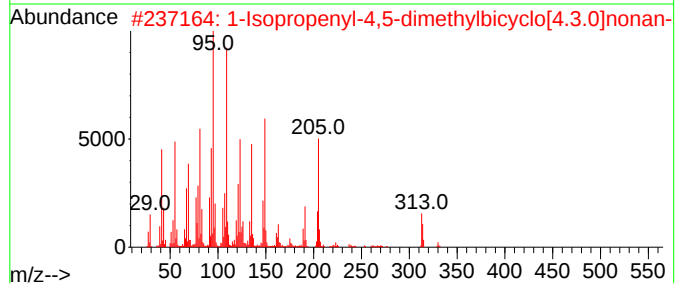
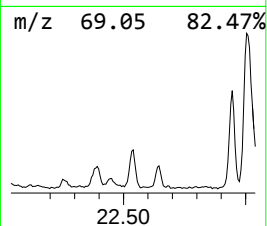
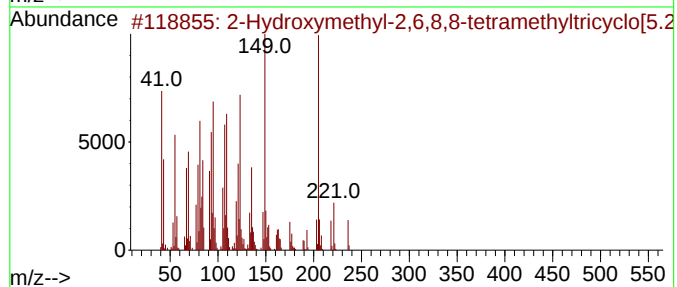
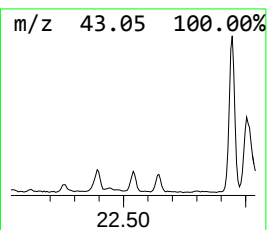
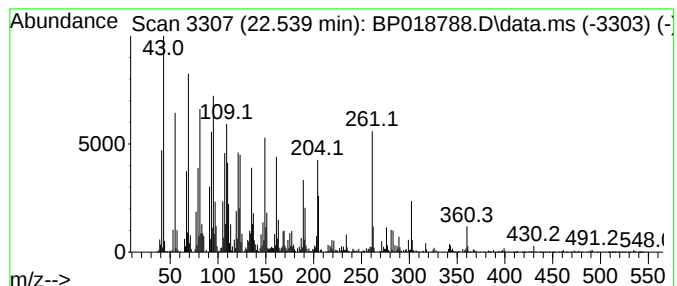
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 2-Hydroxymethyl-2,6,8,8-tet... Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.539	3.39 ng/ul	540949	Perylene-d12	23.663	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxymethyl-2,6,8,8-tetramet...	236	C16H28O	137235-47-3	66
2	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30O5	1000195-85-4	35
3	2-Hydroxy-2,4,4-trimethyl-3-(3-m...	222	C14H22O2	1000191-17-4	27
4	Ledol	222	C15H26O	000577-27-5	22
5	1-Naphthalenol, decahydro-4a-met...	264	C17H28O2	069297-57-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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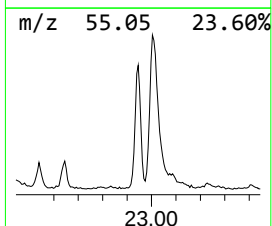
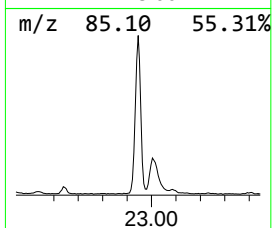
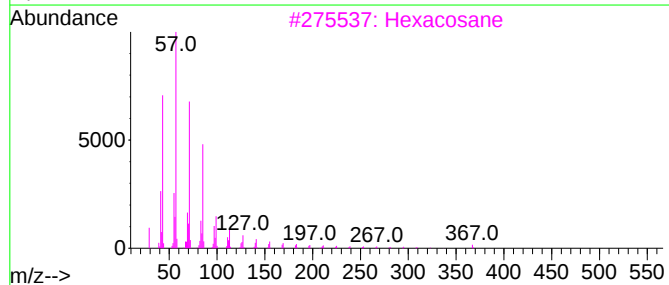
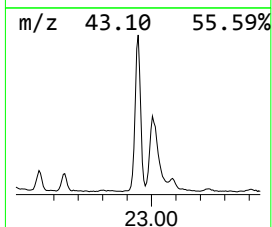
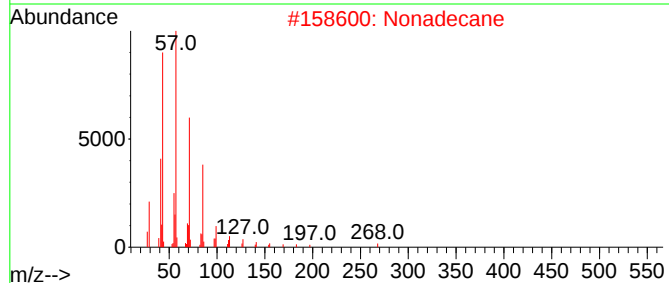
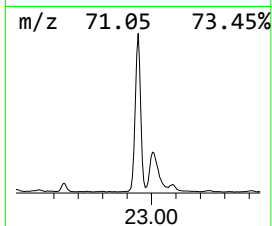
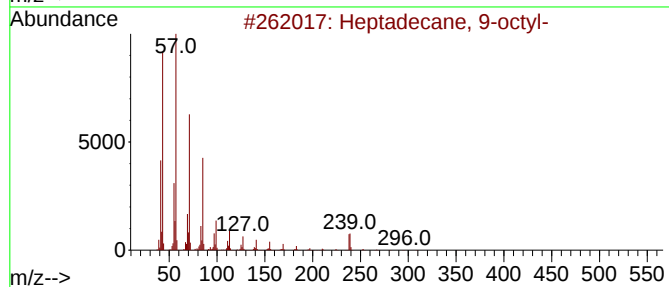
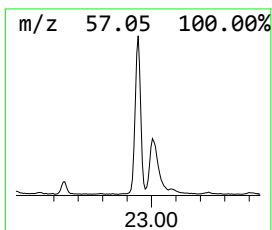
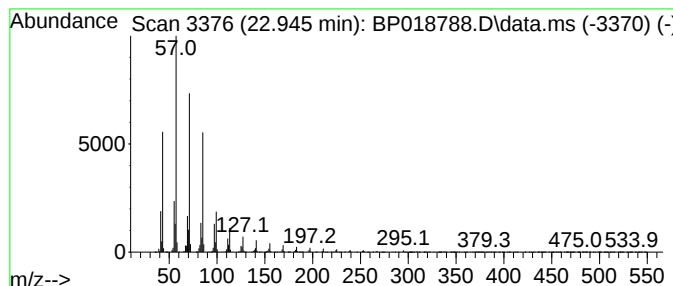
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 (DEL) Alkane: Straight-Chai... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.945	11.79 ng/ul	1879770	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2			Nonadecane	268	C19H40	000629-92-5	94
3			Hexacosane	366	C26H54	000630-01-3	94
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

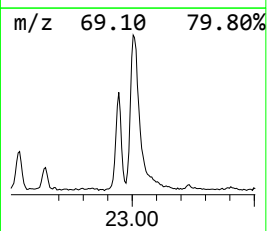
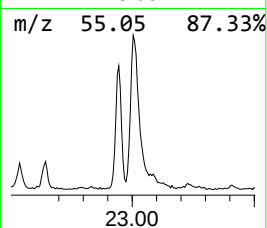
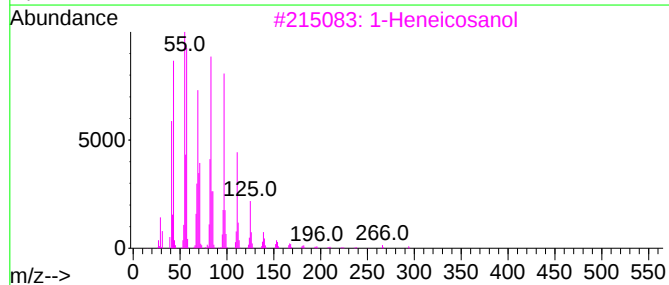
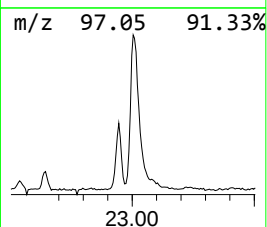
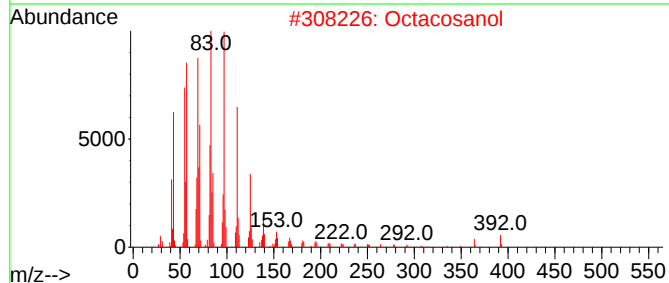
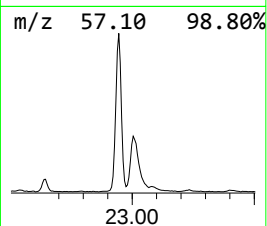
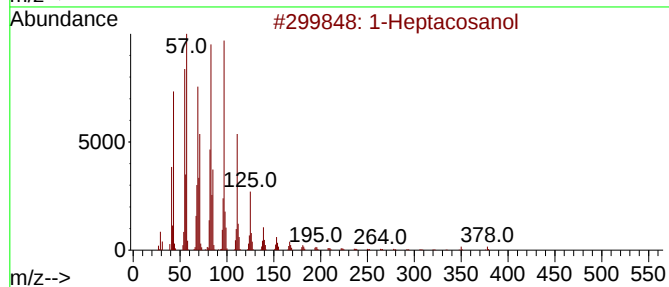
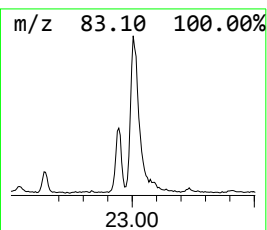
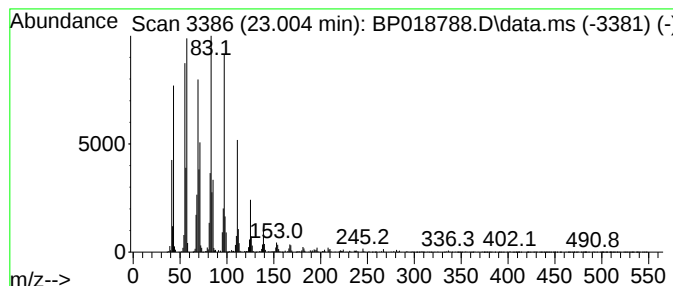
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 1-Heptacosanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.004	12.19 ng/ul	1943840	Perylene-d12	23.663	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Octacosanol	410	C28H58O	000557-61-9	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Nonacos-1-ene	406	C29H58	018835-35-3	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

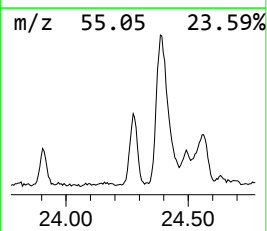
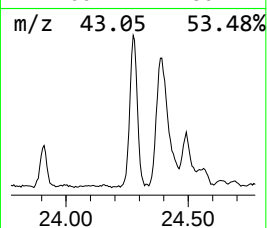
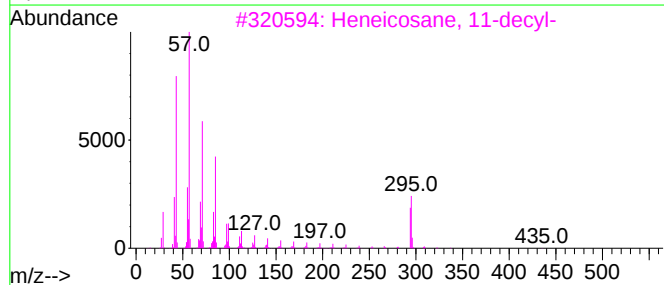
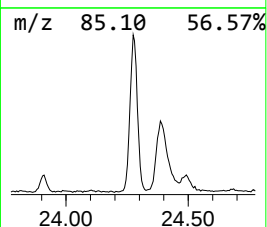
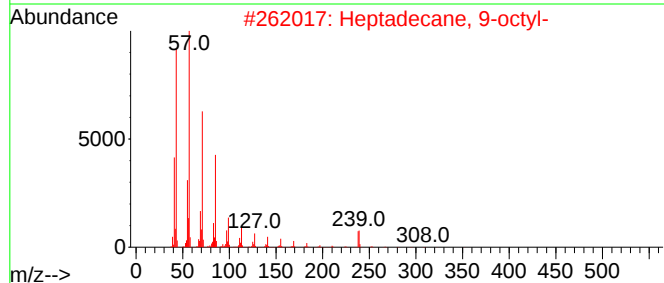
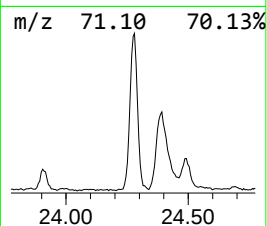
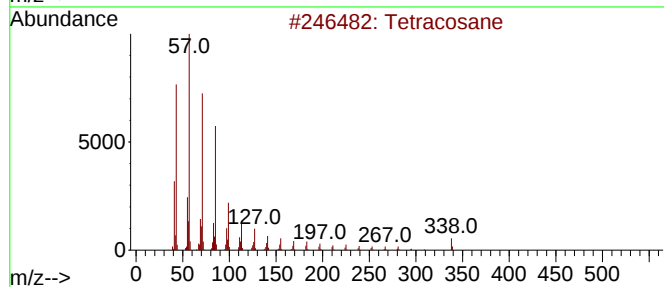
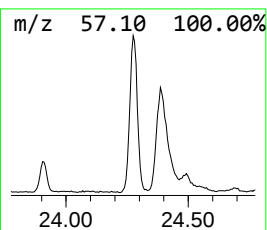
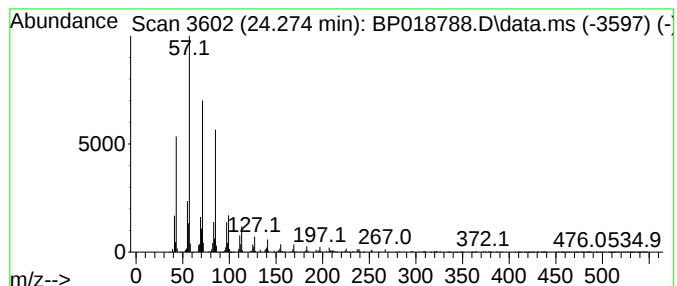
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 (DEL) Alkane: Straight-Chai... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD		R.T.	
24.274	6.08 ng/ul	969057	Perylene-d12		23.663	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetracosane		338	C24H50	000646-31-1	98
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	95
3	Heneicosane, 11-decyl-		437	C31H64	055320-06-4	95
4	Octacosane		394	C28H58	000630-02-4	91
5	Octacosane, 2-methyl-		408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
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Acq On : 13 Dec 2023 03:03
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Misc :
ALS Vial : 67 Sample Multiplier: 1

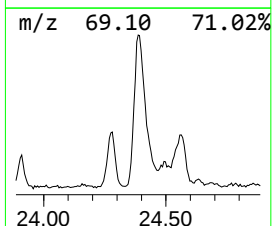
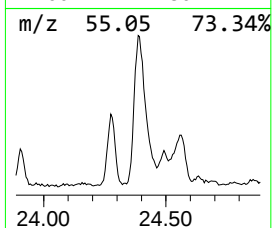
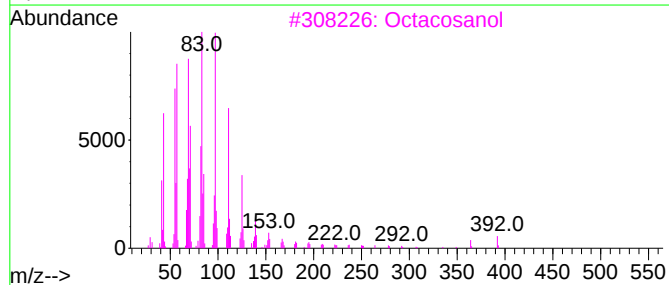
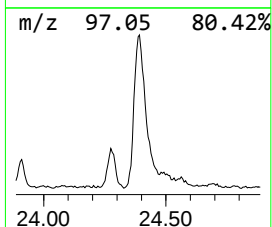
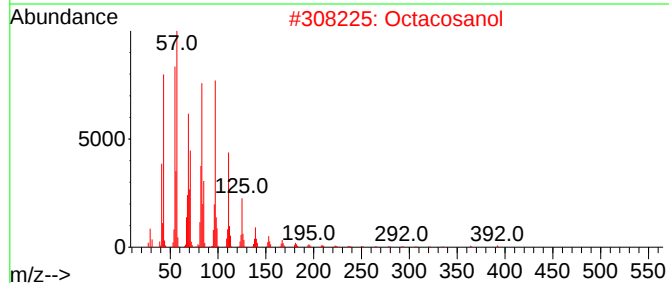
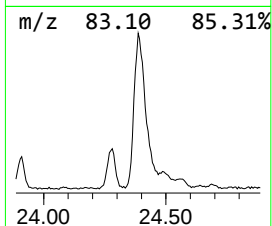
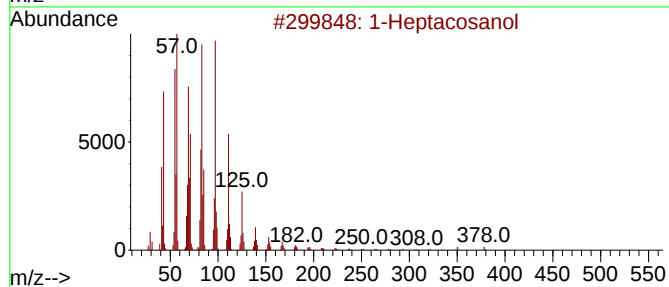
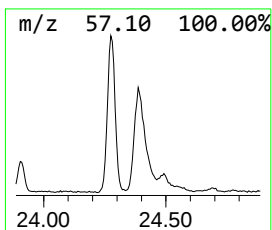
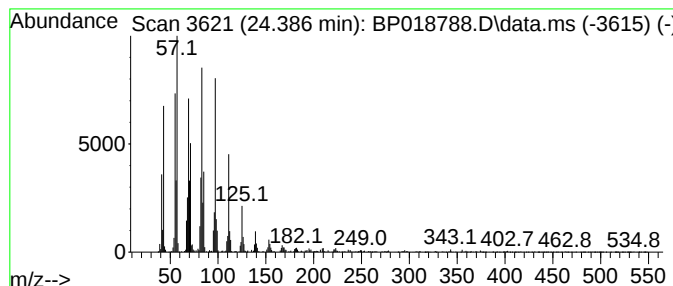
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Octacosanol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.386	10.56 ng/ul	1683640	Perylene-d12	23.663	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Octacosanol	410	C28H58O	000557-61-9	95
3	Octacosanol	410	C28H58O	000557-61-9	95
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5	1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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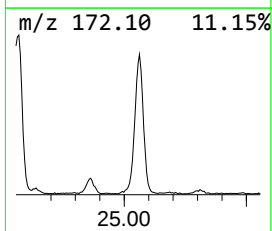
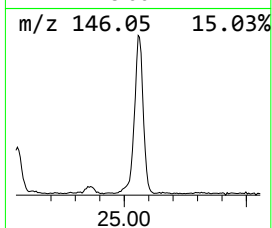
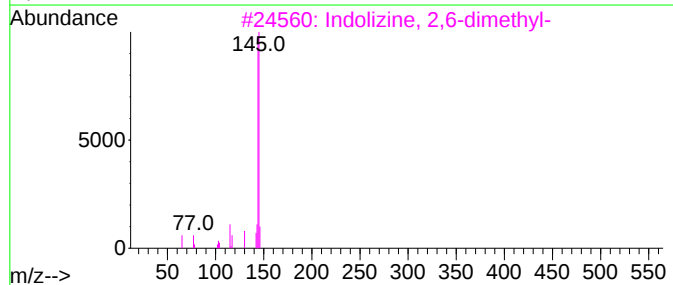
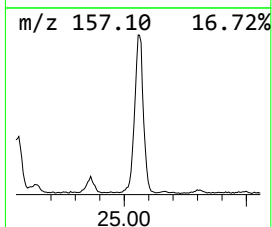
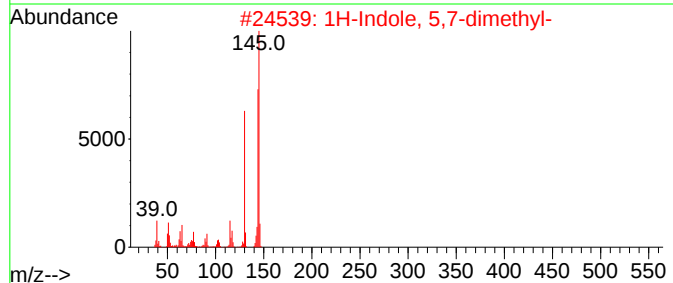
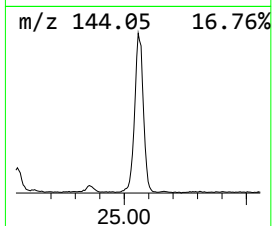
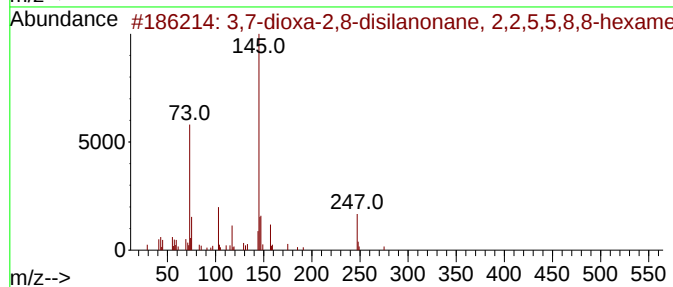
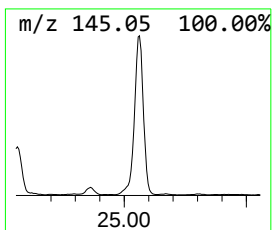
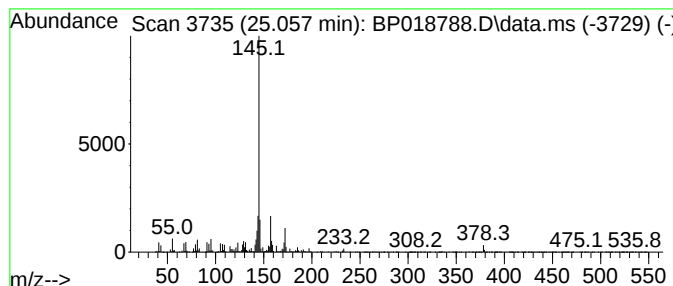
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 3,7-dioxa-2,8-disilanonane,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.057	18.46 ng/ul	2942960	Perylene-d12	23.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-dioxa-2,8-disilanonane, 2,2,...	290	C14H34O2Si2	1000397-32-8	59	
2	1H-Indole, 5,7-dimethyl-	145	C10H11N	054020-53-0	53	
3	Indolizine, 2,6-dimethyl-	145	C10H11N	000769-88-0	53	
4	1H-Indole, 2,5-dimethyl-	145	C10H11N	001196-79-8	53	
5	Indole, 1,7-dimethyl-	145	C10H11N	005621-16-9	53	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AY7

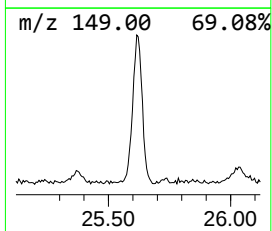
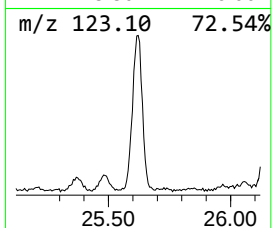
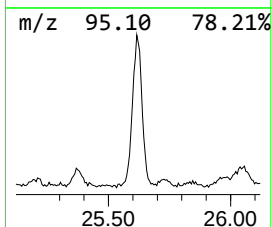
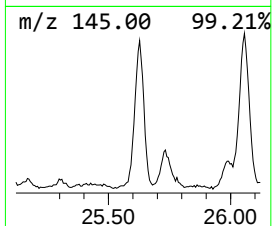
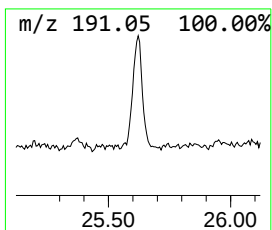
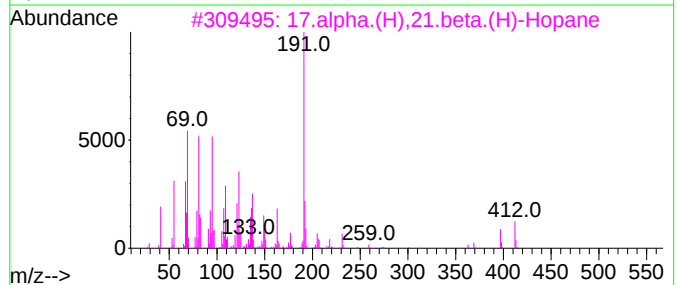
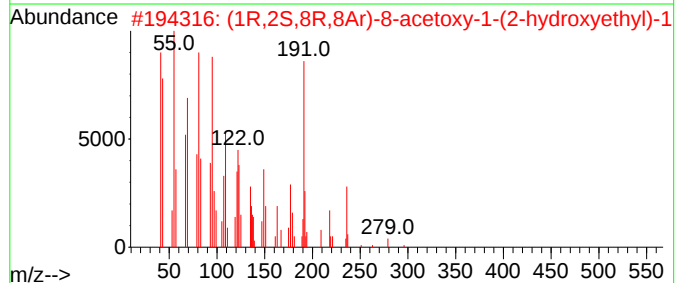
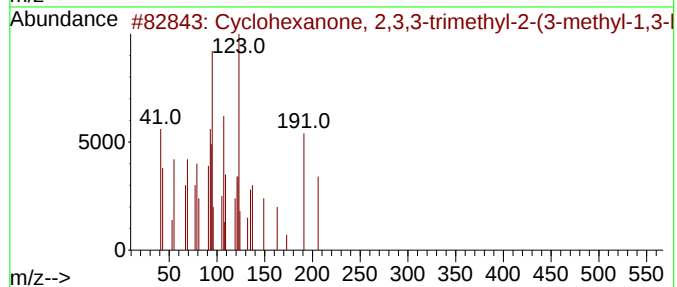
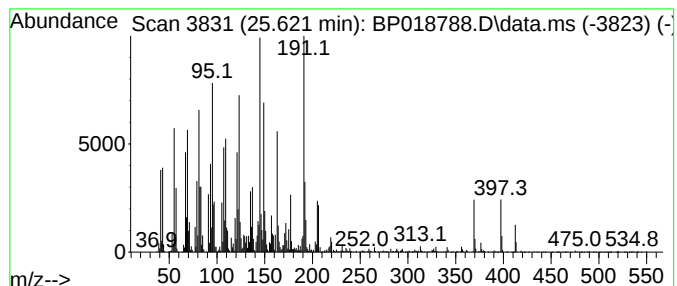
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown-04 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.621	12.50 ng/ul	1993340	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	52
2			(1R,2S,8R,8Ar)-8-acetoxy-1-(2-hy...	296	C18H32O3	1000298-98-4	38
3			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	38
4			2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	35
5			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AY7

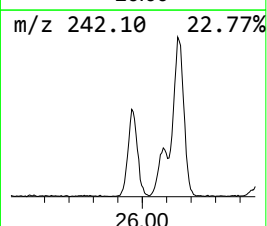
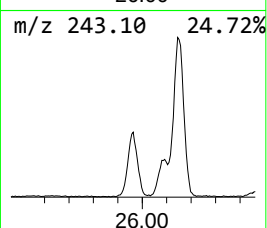
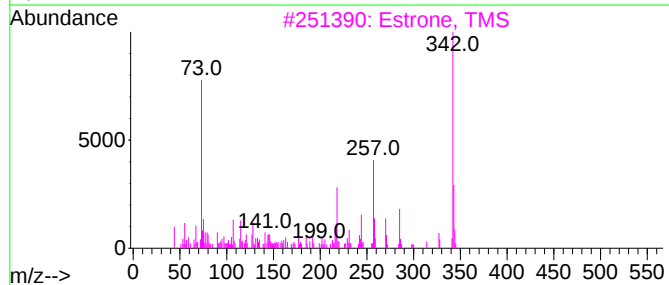
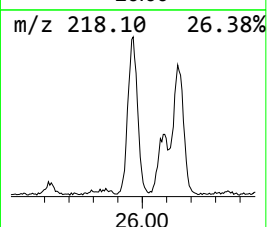
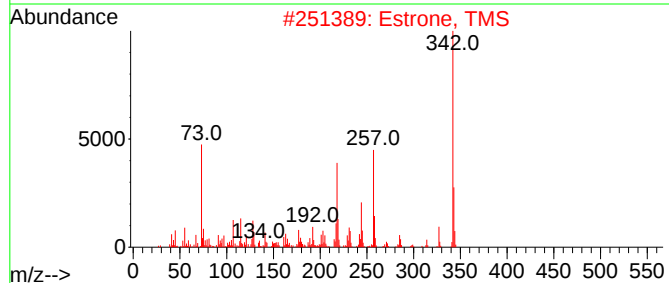
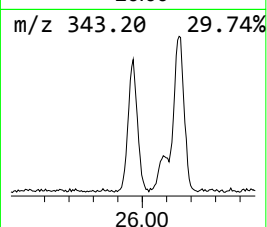
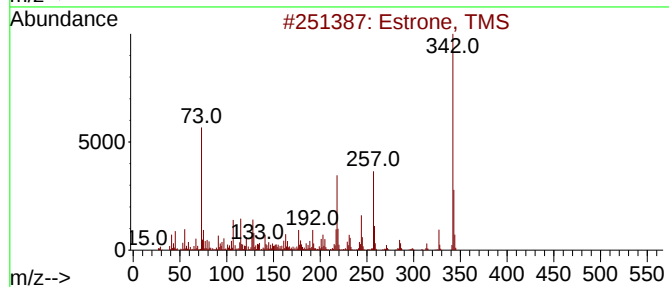
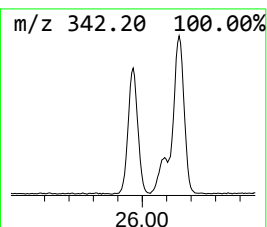
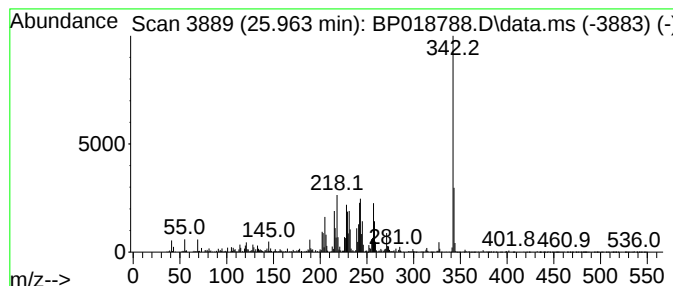
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 21 Estrone, TMS Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.963	6.47 ng/ul	1030910	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Estrone, TMS	342	C21H30O2Si	001839-54-9	50
2			Estrone, TMS	342	C21H30O2Si	001839-54-9	47
3			Estrone, TMS	342	C21H30O2Si	001839-54-9	37
4			4,6-Bis(1,1'-dimethylethyl)-2',5...	342	C22H30O3	1000326-27-3	35
5			4H-1-Benzopyran-4-one, 3-(3,4-di...	342	C19H18O6	024126-93-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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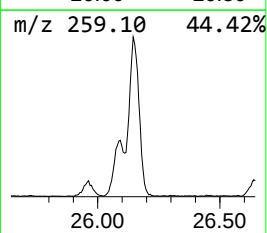
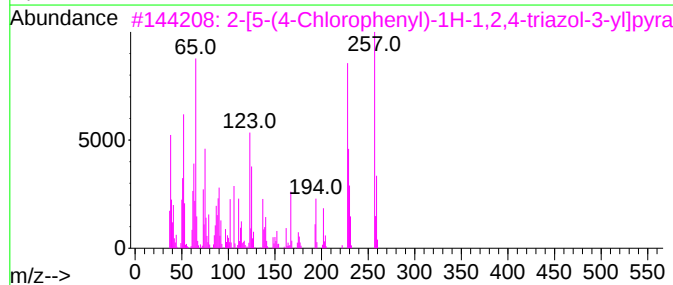
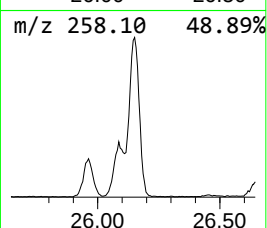
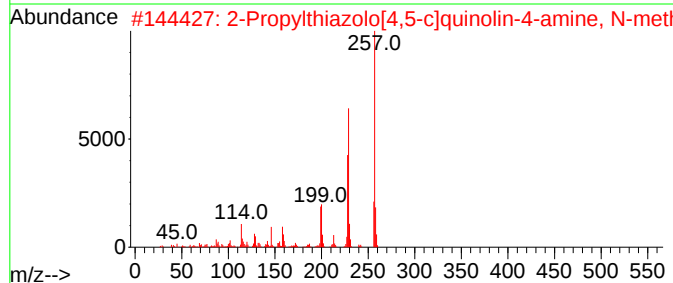
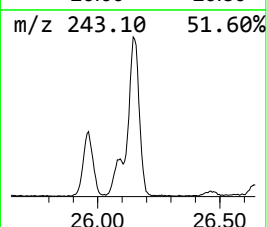
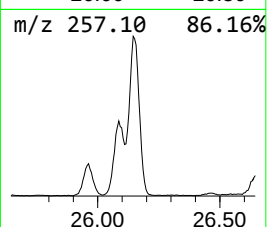
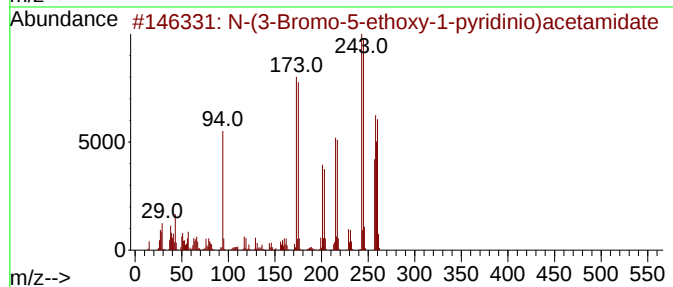
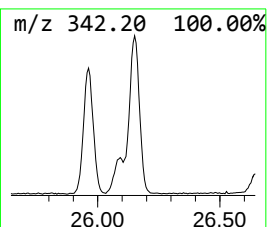
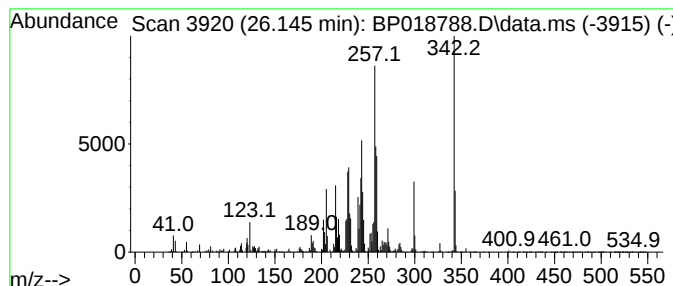
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 22 unknown-05 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.145	16.32 ng/ul	2602290	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(3-Bromo-5-ethoxy-1-pyridinio)...	258	C9H11BrN2O2	035990-11-5	25
2			2-Propylthiazolo[4,5-c]quinolin-...	257	C14H15N3S	1000499-65-1	25
3			2-[5-(4-Chlorophenyl)-1H-1,2,4-t...	257	C12H8ClN5	1000387-00-3	14
4			1H,6H-5,11b-Ethano[1,3]dioxolo[4...	257	C16H19N02	000510-70-3	14
5			4-(Hydroxyimino)-3-(4-methylphen...	257	C14H15N3O2	1000444-47-4	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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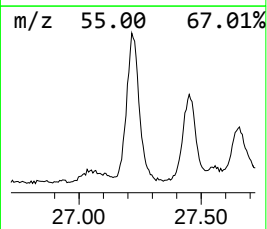
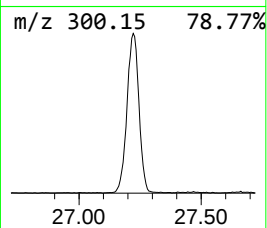
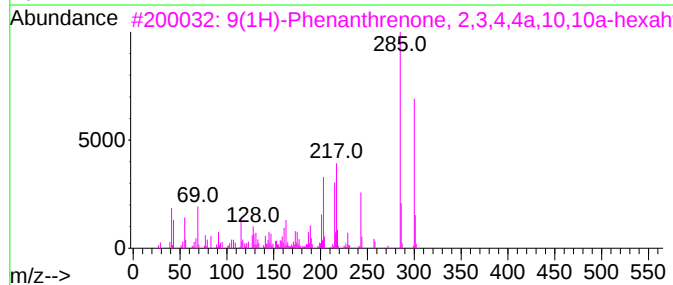
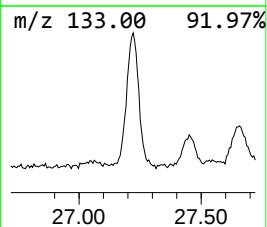
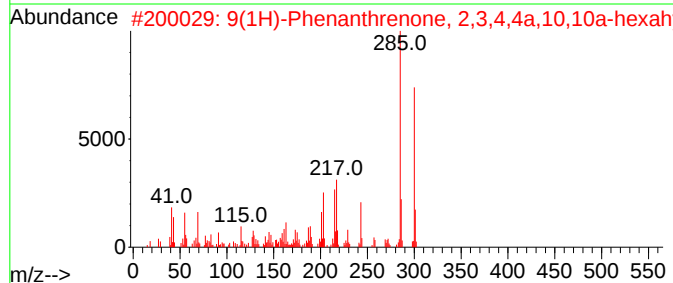
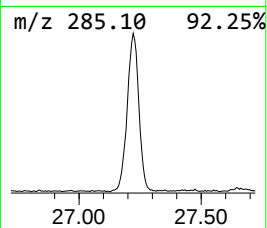
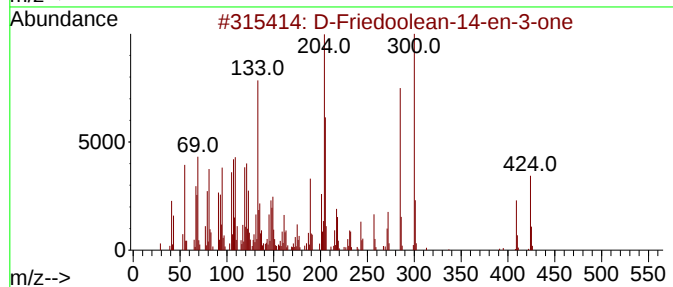
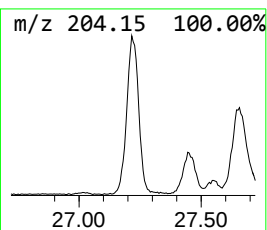
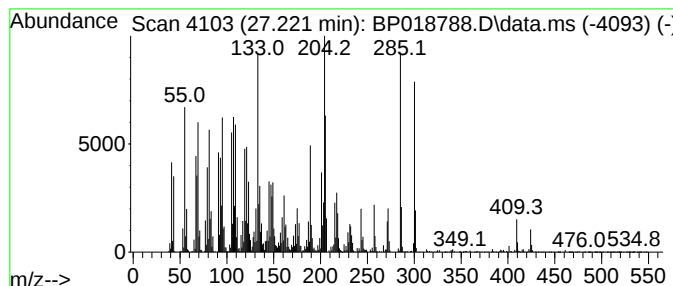
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 23 D-Friedoolean-14-en-3-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.221	33.44 ng/ul	5332090	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Friedoolean-14-en-3-one	424	C30H48O	000514-07-8	93
2			9(1H)-Phenanthrene, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	86
3			9(1H)-Phenanthrene, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	66
4			Estra-1,3,5(10)-trien-17-one, 3-...	300	C19H24O3	000362-08-3	59
5			4H-1-Benzopyran-4-one, 3,7-dihyd...	300	C16H12O6	057396-72-2	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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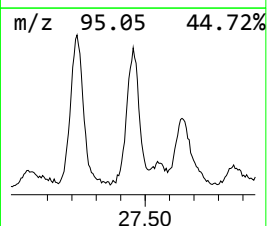
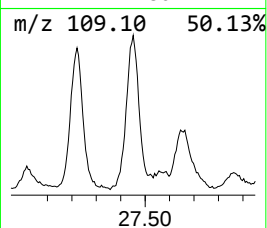
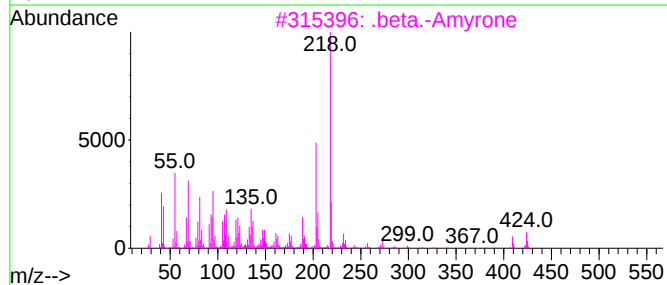
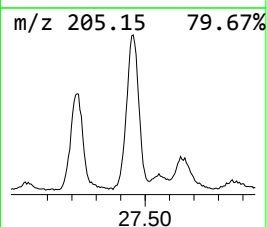
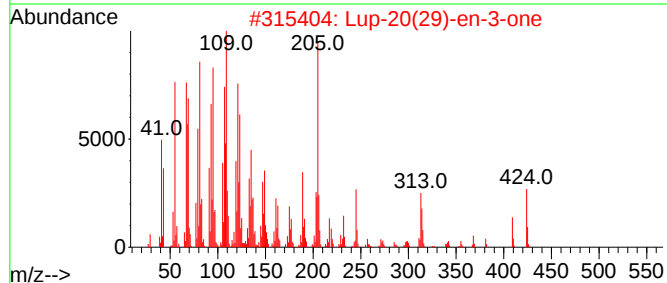
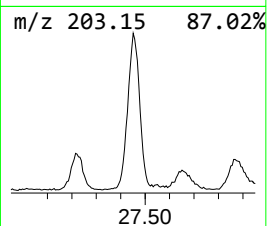
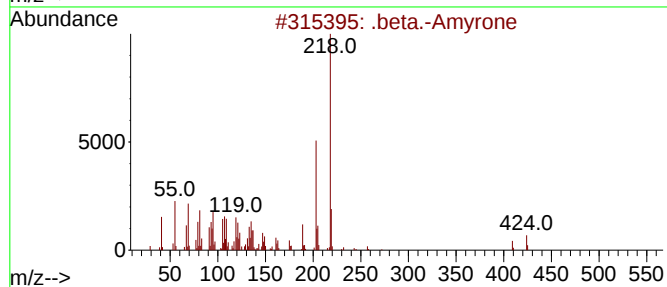
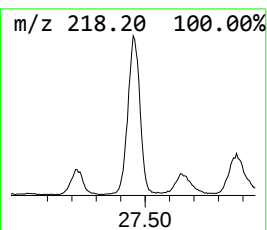
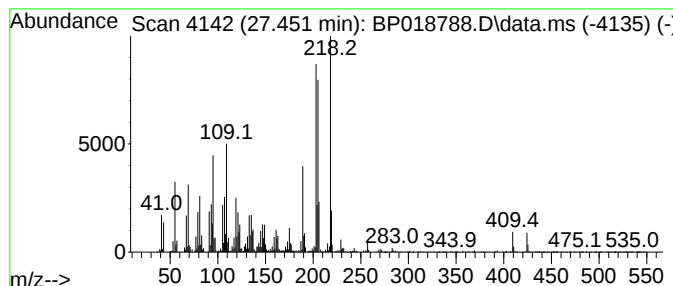
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 24 .beta.-Amyrone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.451	14.25 ng/ul	2271310	Perylene-d12	23.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Amyrone	424	C30H48O	000638-97-1	86
2		Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	83
3		.beta.-Amyrone	424	C30H48O	000638-97-1	60
4		D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	38
5		Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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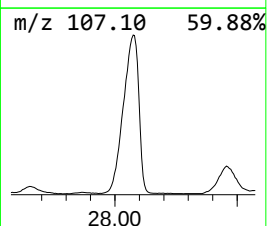
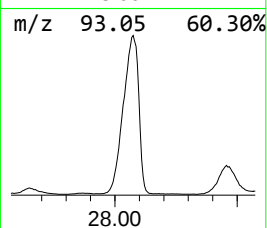
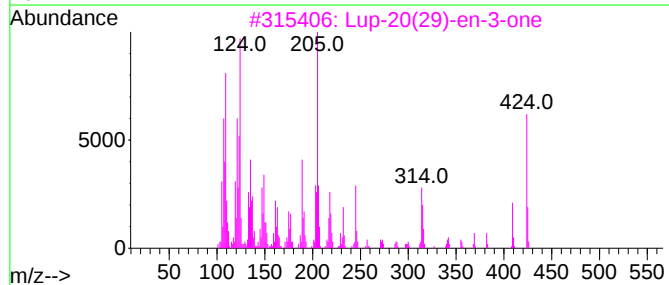
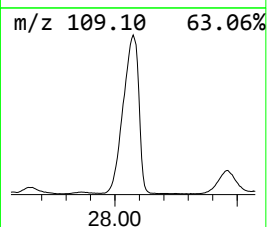
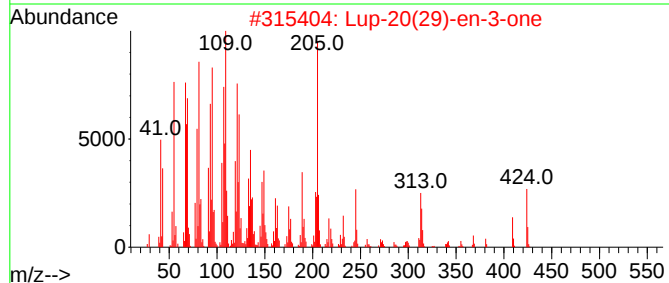
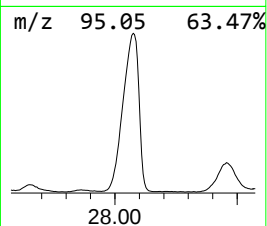
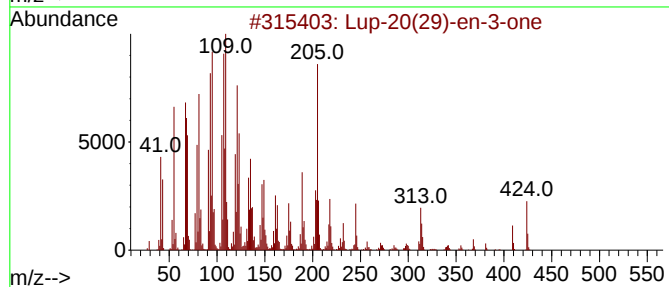
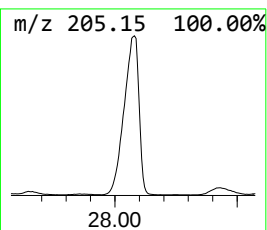
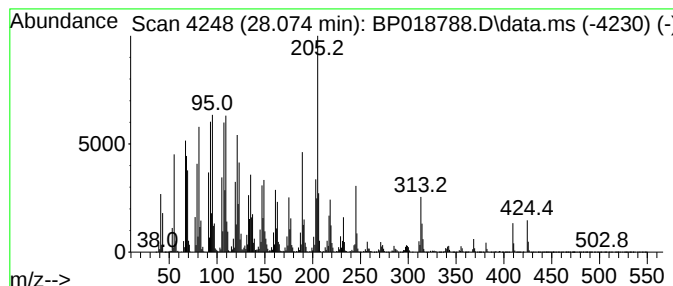
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 25 Lup-20(29)-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.074	305.81 ng/ul	48757400	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
3			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	94
4			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	92
5			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018788.D
Acq On : 13 Dec 2023 03:03
Operator : MA/JU
Sample : 05646-11
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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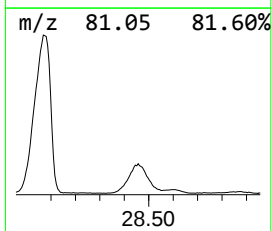
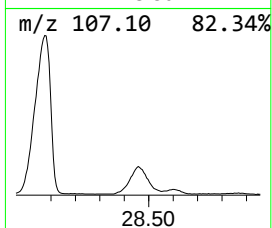
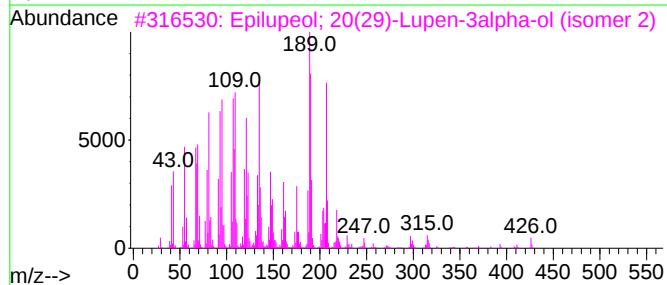
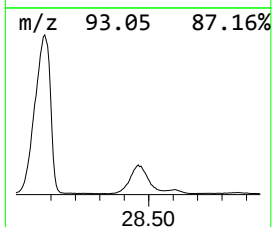
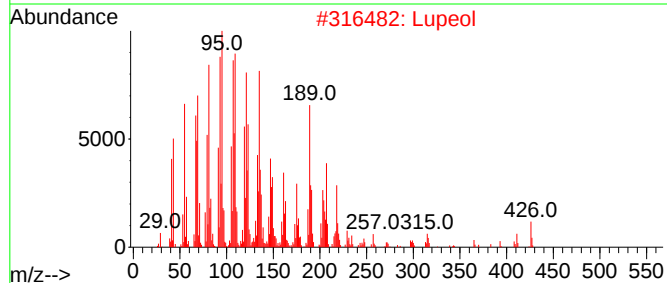
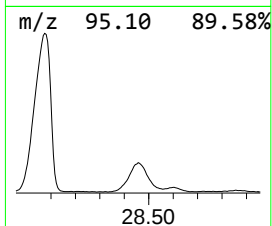
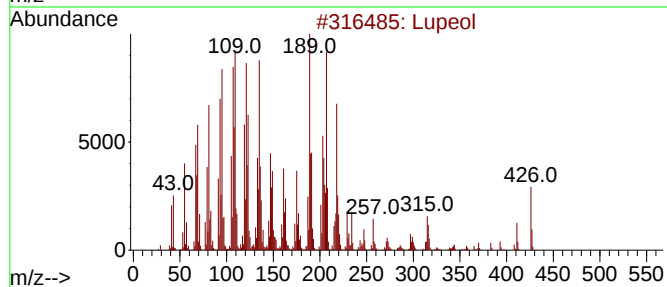
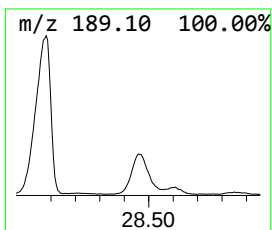
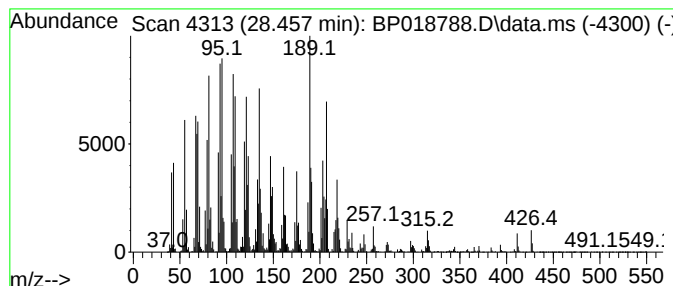
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 26 Lupeol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.457	49.79 ng/ul	7938680	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	99
2			Lupeol	426	C30H50O	000545-47-1	95
3			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	86
4			Taraxasterol	426	C30H50O	001059-14-9	86
5			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
 Data File : BP018788.D
 Acq On : 13 Dec 2023 03:03
 Operator : MA/JU
 Sample : 05646-11
 Misc :
 ALS Vial : 67 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AY7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
 Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzoic acid	9.887	2.9	ng/ul	185355	2	10.634	1300730	20.0
n-Hexadecanoic ...	18.104	3.0	ng/ul	345949	4	17.216	2343950	20.0
unknown-01	19.128	2.2	ng/ul	262979	4	17.216	2343950	20.0
unknown-02	20.728	12.5	ng/ul	2096600	5	21.304	3350470	20.0
Cycloheptane, 4...	20.798	2.2	ng/ul	366611	5	21.304	3350470	20.0
2-Butenal, 2-me...	20.916	47.4	ng/ul	7944120	5	21.304	3350470	20.0
unknown-03	20.957	3.0	ng/ul	508318	5	21.304	3350470	20.0
Ethanol, 2-(tet...	21.022	9.4	ng/ul	1568920	5	21.304	3350470	20.0
Cyclohexanone, ...	21.051	26.6	ng/ul	4460750	5	21.304	3350470	20.0
(DEL) Alkane: S...	21.904	4.1	ng/ul	687470	5	21.304	3350470	20.0
1-Heneicosanol	21.933	11.1	ng/ul	1857950	5	21.304	3350470	20.0
2-Hydroxymethyl...	22.539	3.4	ng/ul	540949	6	23.663	3188780	20.0
(DEL) Alkane: S...	22.945	11.8	ng/ul	1879770	6	23.663	3188780	20.0
1-Heptacosanol	23.004	12.2	ng/ul	1943840	6	23.663	3188780	20.0
(DEL) Alkane: S...	24.274	6.1	ng/ul	969057	6	23.663	3188780	20.0
Octacosanol	24.386	10.6	ng/ul	1683640	6	23.663	3188780	20.0
3,7-dioxa-2,8-d...	25.057	18.5	ng/ul	2942960	6	23.663	3188780	20.0
unknown-04	25.621	12.5	ng/ul	1993340	6	23.663	3188780	20.0
Estrone, TMS	25.963	6.5	ng/ul	1030910	6	23.663	3188780	20.0
unknown-05	26.145	16.3	ng/ul	2602290	6	23.663	3188780	20.0
D-Friedoolean-1...	27.221	33.4	ng/ul	5332090	6	23.663	3188780	20.0
.beta.-Amyrone	27.451	14.3	ng/ul	2271310	6	23.663	3188780	20.0
Lup-20(29)-en-3...	28.074	305.8	ng/ul	48757400	6	23.663	3188780	20.0
Lupeol	28.457	49.8	ng/ul	7938680	6	23.663	3188780	20.0