

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
 Data File : BP018172.D
 Acq On : 15 Nov 2023 00:37
 Operator : MA/JU
 Sample : 05158-01
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BH362

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-BP111023.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018172.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.164	9	13	18	rVB	13277	16037	0.34%	0.043%
2	3.611	86	89	101	rBV	33292	76496	1.61%	0.207%
3	3.711	104	106	113	rVB8	6904	10932	0.23%	0.030%
4	3.781	113	118	121	rBV5	5499	7033	0.15%	0.019%
5	3.899	135	138	142	rBV4	5093	7419	0.16%	0.020%
6	5.328	377	381	388	rVB6	10221	15778	0.33%	0.043%
7	6.964	653	659	678	rBV2	48893	123504	2.60%	0.334%
8	7.140	683	689	701	rBV	209611	352090	7.42%	0.952%
9	7.311	710	718	731	rBV	219594	394582	8.32%	1.067%
10	7.787	793	799	811	rBV	263091	447493	9.44%	1.210%
11	8.516	916	923	938	rBV	150193	310896	6.56%	0.841%
12	8.993	997	1004	1018	rBV	266973	490501	10.34%	1.326%
13	9.163	1029	1033	1041	rVB	33653	49171	1.04%	0.133%
14	9.705	1119	1125	1141	rBV	217941	424015	8.94%	1.146%
15	9.887	1152	1156	1159	rVB5	3130	4984	0.11%	0.013%
16	10.234	1209	1215	1235	rBV2	246580	567749	11.97%	1.535%
17	10.605	1271	1278	1290	rVB	356849	600920	12.67%	1.625%
18	10.787	1302	1309	1330	rBV	199027	491772	10.37%	1.330%
19	12.222	1550	1553	1563	rBV	4353	9880	0.21%	0.027%
20	12.781	1642	1648	1650	rBV7	2383	4770	0.10%	0.013%
21	13.310	1733	1738	1747	rVB6	10749	21405	0.45%	0.058%
22	13.887	1830	1836	1842	rBV	753572	1039753	21.92%	2.811%
23	13.934	1842	1844	1853	rVB	19216	31845	0.67%	0.086%
24	14.087	1865	1870	1877	rBV10	2433	6719	0.14%	0.018%
25	14.163	1877	1883	1891	rBV2	712494	1050832	22.16%	2.841%
26	14.463	1928	1934	1946	rBV	530000	787147	16.60%	2.128%
27	14.787	1983	1989	2000	rBV6	15432	54774	1.15%	0.148%
28	14.981	2014	2022	2027	rVB6	3213	6993	0.15%	0.019%
29	15.469	2099	2105	2115	rBV	1013840	1426784	30.08%	3.858%
30	15.628	2127	2132	2144	rBV	227337	403981	8.52%	1.092%
31	16.122	2210	2216	2222	rBV	3527	6661	0.14%	0.018%
32	16.269	2237	2241	2246	rVB8	2833	5293	0.11%	0.014%
33	16.339	2249	2253	2258	rVB8	3682	6995	0.15%	0.019%
34	16.739	2316	2321	2326	rBV4	7211	12353	0.26%	0.033%
35	17.039	2369	2372	2378	rVB7	3717	5813	0.12%	0.016%
36	17.128	2382	2387	2396	rVB7	5967	11280	0.24%	0.030%

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37	17.210	2396	2401	2402	rBV4	28557	31092	0.66%	0.084%
38	17.245	2402	2407	2418	rVB	738667	997633	21.03%	2.697%
39	17.345	2418	2424	2438	rBV2	1161852	1643306	34.65%	4.443%
40	17.534	2454	2456	2460	rVB4	9516	11716	0.25%	0.032%
41	17.875	2511	2514	2518	rVB6	7413	9001	0.19%	0.024%
42	18.098	2547	2552	2559	rBV	77287	112691	2.38%	0.305%
43	18.192	2564	2568	2576	rVB	61468	81956	1.73%	0.222%
44	18.516	2619	2623	2629	rVB4	44801	52122	1.10%	0.141%
45	18.586	2630	2635	2642	rVV	121437	142816	3.01%	0.386%
46	18.663	2646	2648	2654	rVV6	7498	9695	0.20%	0.026%
47	18.769	2663	2666	2669	rVB5	6914	8475	0.18%	0.023%
48	19.175	2732	2735	2739	rBV2	14761	19496	0.41%	0.053%
49	19.251	2744	2748	2752	rVB	15827	21700	0.46%	0.059%
50	19.345	2760	2764	2771	rBV7	22181	36791	0.78%	0.099%
51	19.480	2784	2787	2790	rBV4	10419	10463	0.22%	0.028%
52	19.604	2802	2808	2815	rBV	1776009	2168582	45.72%	5.864%
53	19.898	2855	2858	2862	rVB6	11890	13838	0.29%	0.037%
54	20.186	2905	2907	2910	rBV4	8405	8830	0.19%	0.024%
55	21.039	3047	3052	3062	rBV3	104381	248779	5.25%	0.673%
56	21.375	3104	3109	3117	rBV	917597	1199144	25.28%	3.242%
57	21.751	3170	3173	3176	rVB3	45127	46408	0.98%	0.125%
58	21.851	3187	3190	3194	rVB2	102121	119883	2.53%	0.324%
59	21.898	3195	3198	3201	rVV3	68688	73978	1.56%	0.200%
60	22.016	3213	3218	3221	rBV	209872	266848	5.63%	0.722%
61	22.110	3230	3234	3248	rVB	673992	870665	18.36%	2.354%
62	22.239	3250	3256	3262	rBV	3578522	4742859	100.00%	12.824%
63	22.510	3297	3302	3310	rVB	1198401	1780188	37.53%	4.813%
64	22.757	3335	3344	3354	rVB2	581862	1071358	22.59%	2.897%
65	22.933	3369	3374	3383	rVB2	155153	270387	5.70%	0.731%
66	23.033	3384	3391	3399	rVB	2856018	4463372	94.11%	12.068%
67	23.221	3417	3423	3430	rBV2	1274968	2388318	50.36%	6.458%
68	23.539	3472	3477	3481	rBV3	120908	201082	4.24%	0.544%
69	23.592	3482	3486	3492	rVB4	114985	191954	4.05%	0.519%
70	23.680	3494	3501	3512	rVB2	1409233	3000906	63.27%	8.114%
71	23.845	3522	3529	3541	rVB	677187	1383356	29.17%	3.740%

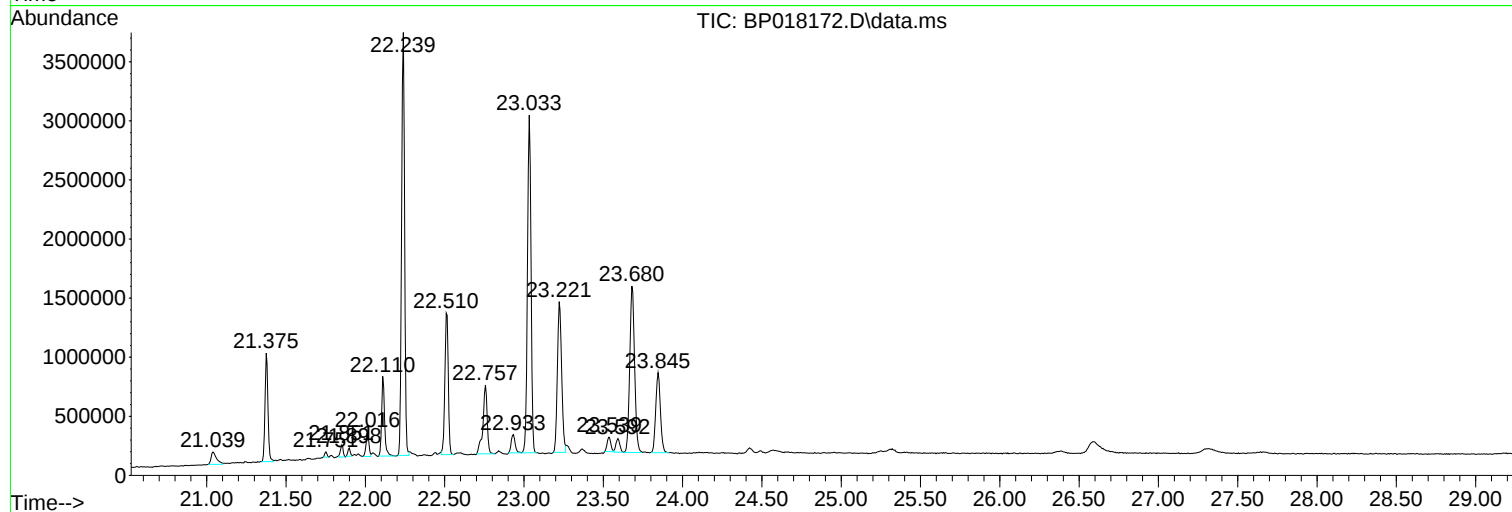
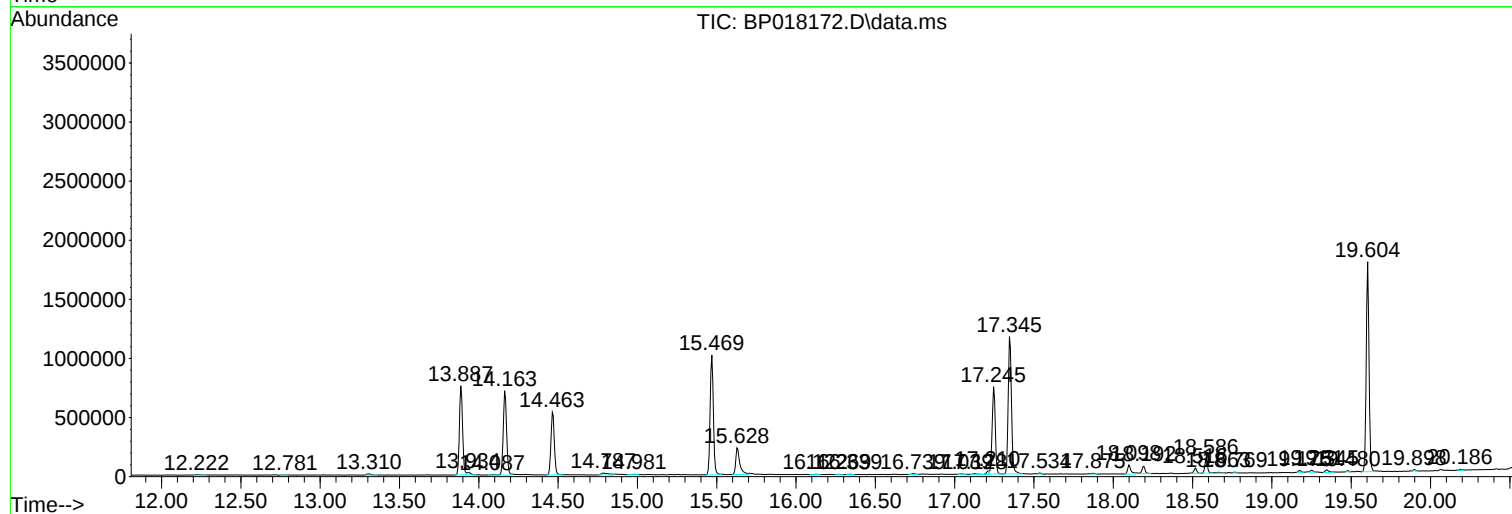
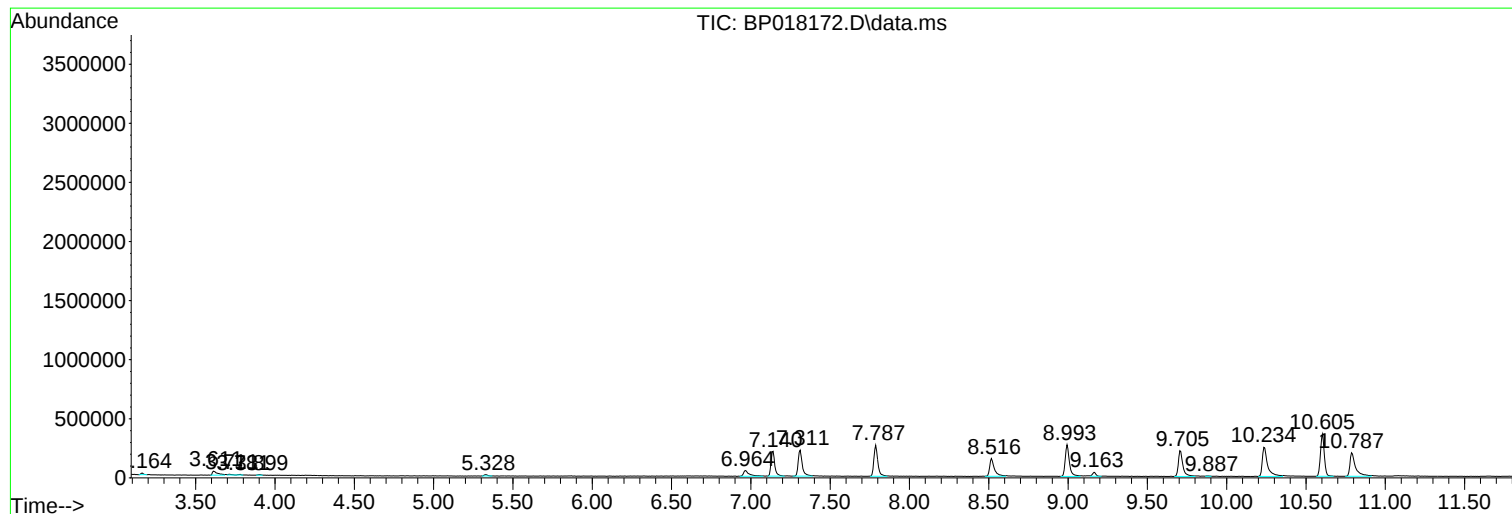
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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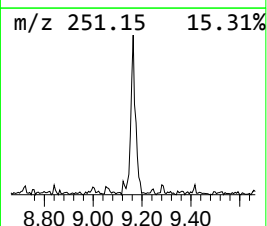
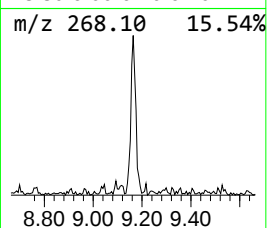
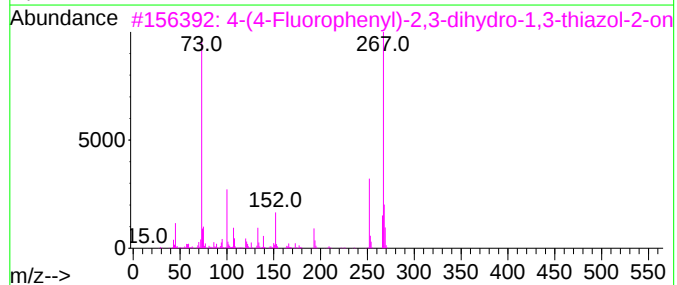
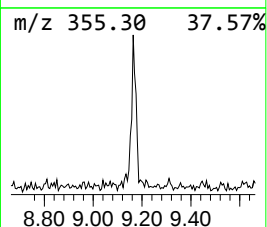
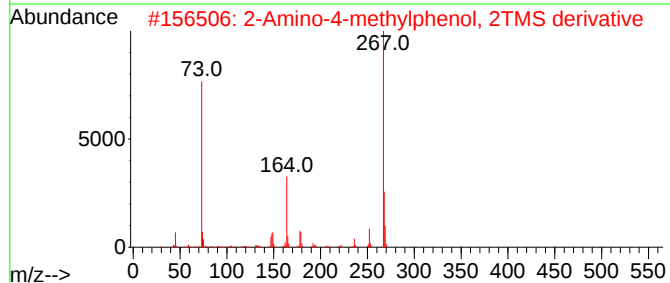
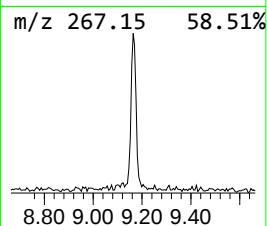
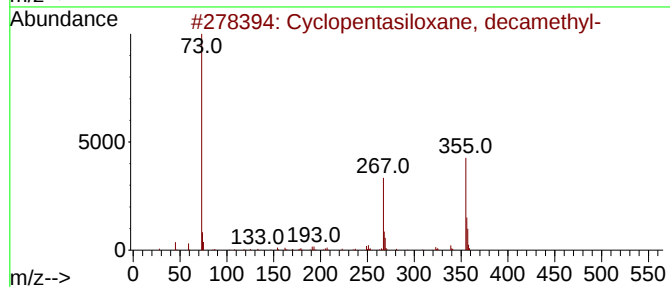
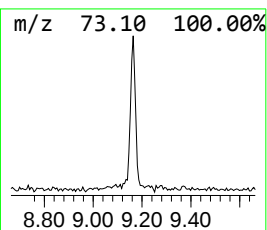
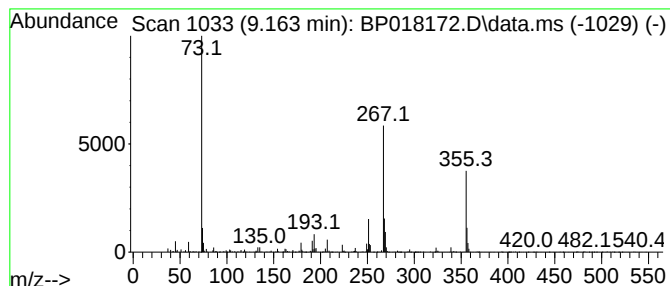
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Cyclopentasiloxane, decamet... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.163	2.20 ng/ul	49171	1,4-Dichlorobenzene-d4	7.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	72
2			2-Amino-4-methylphenol, 2TMS der...	267	C13H25NOSi2	1000373-28-1	50
3			4-(4-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSi	1010501-61-0	49
4			4-(2-amino-1-hydroxypropyl)pheno...	311	C15H29NO2Si2	1000478-98-6	49
5			Trimethylsilyl catechollactate t...	486	C21H42O5Si4	068595-72-2	47



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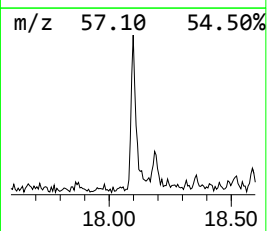
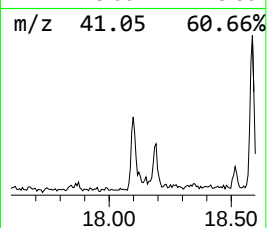
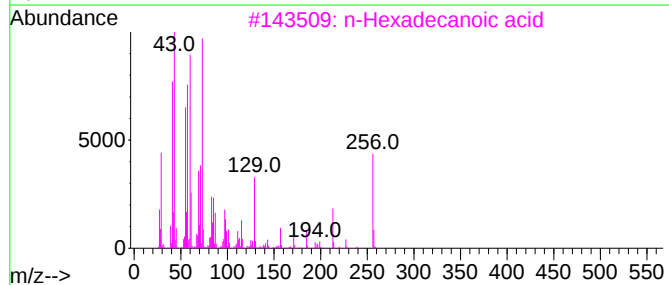
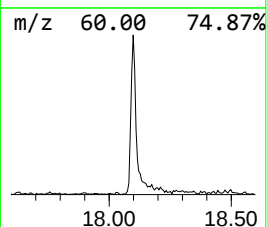
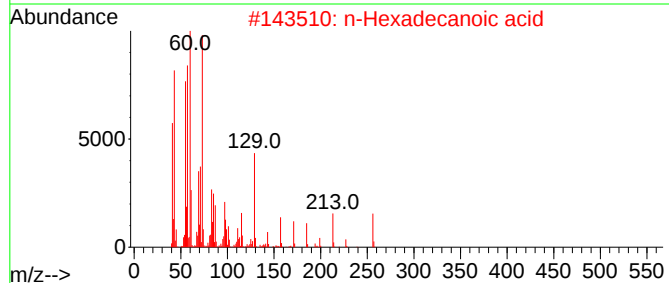
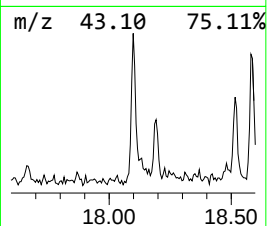
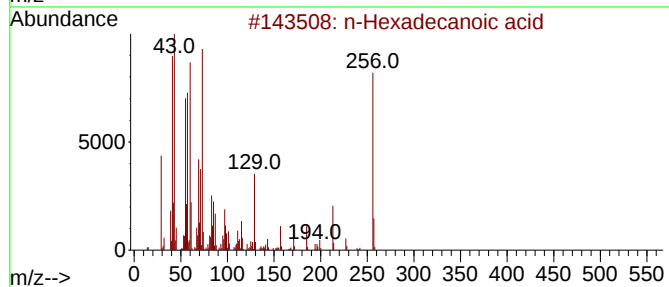
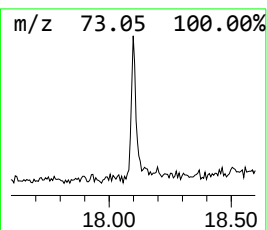
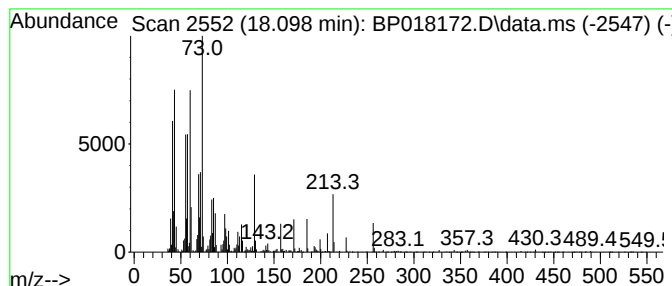
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	2.26 ng/ul	112691	Phenanthrene-d10	17.245

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	98		
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98		
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90		
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81		



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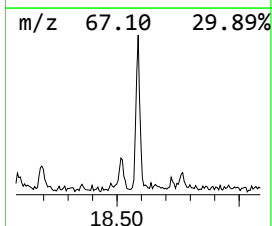
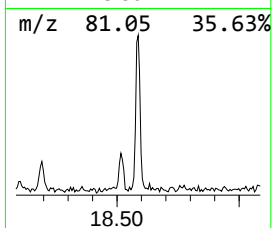
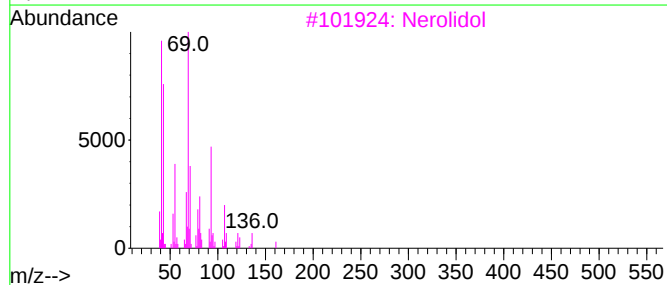
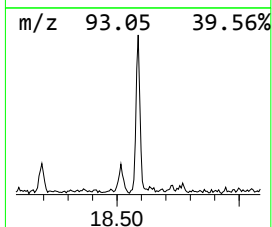
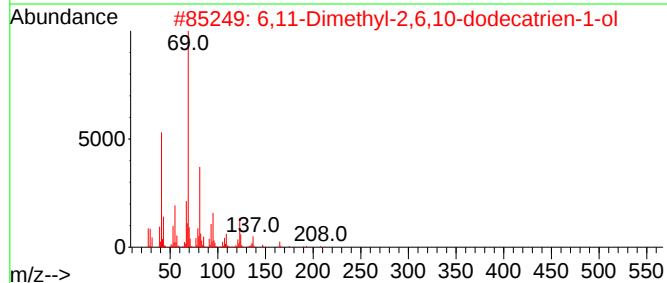
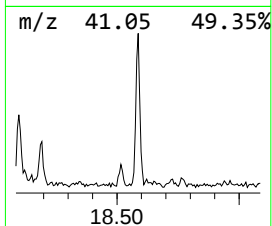
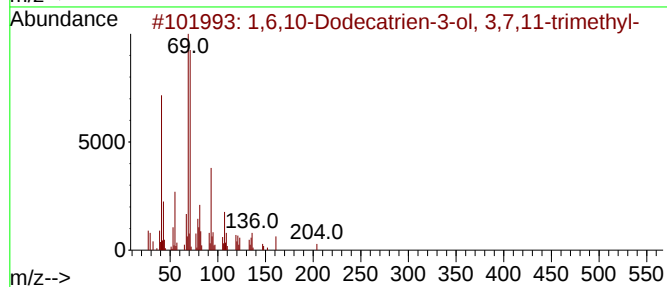
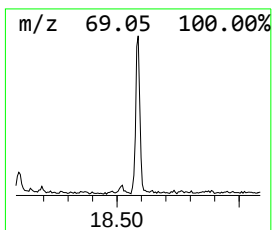
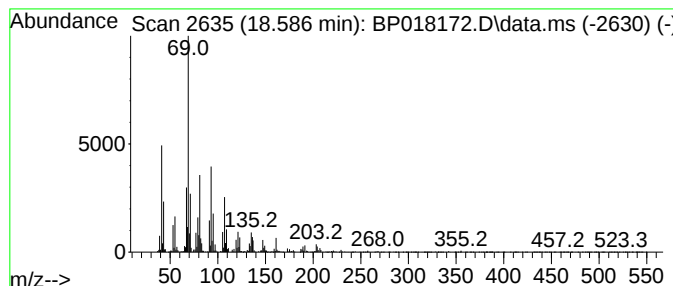
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Peak Number 3 1,6,10-Dodecatrien-3-ol, 3,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.586	2.86 ng/ul	142816	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,10-Dodecatrien-3-ol, 3,7,11-...	222	C15H26O	007212-44-4	62		
2	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	60		
3	Nerolidol	222	C15H26O	000142-50-7	59		
4	1,6,10,14,18,22-Tetracosahexaen...	426	C30H50O	097232-74-1	58		
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	53		



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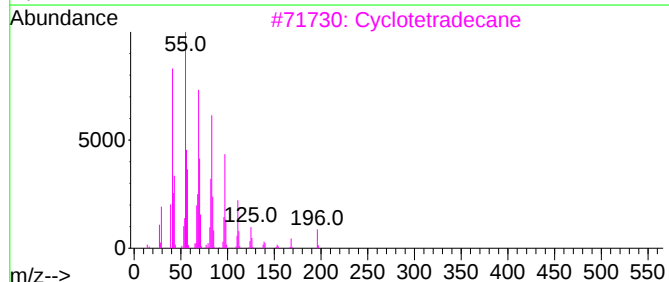
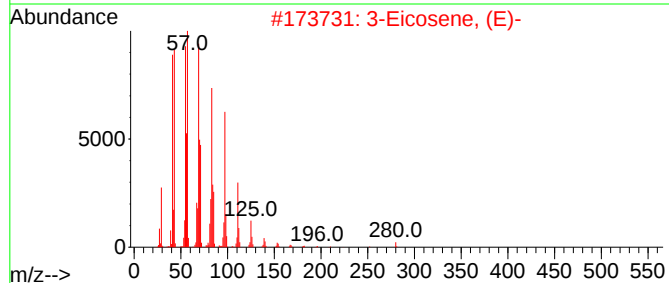
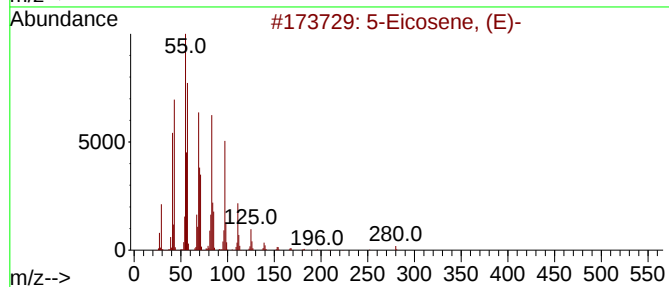
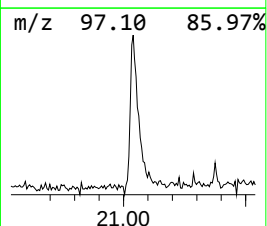
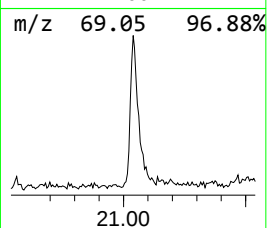
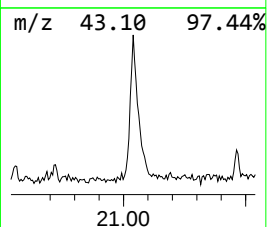
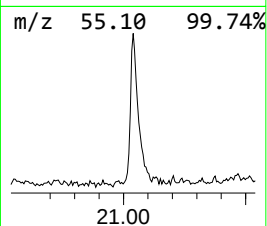
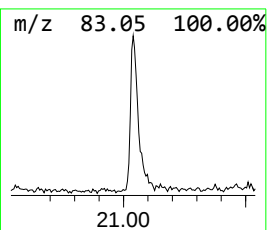
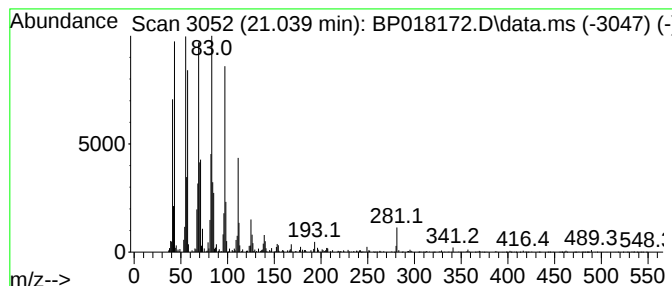
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.039	4.15 ng/ul	248779	Chrysene-d12	21.375

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3		Cyclotetradecane	196	C14H28	000295-17-0	96
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
Data File : BP018172.D
Acq On : 15 Nov 2023 00:37
Operator : MA/JU
Sample : 05158-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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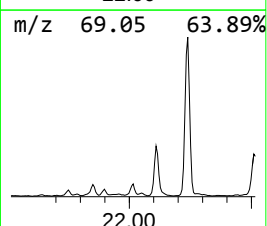
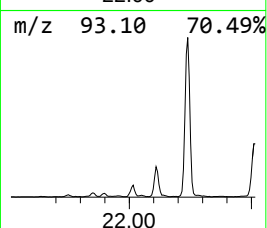
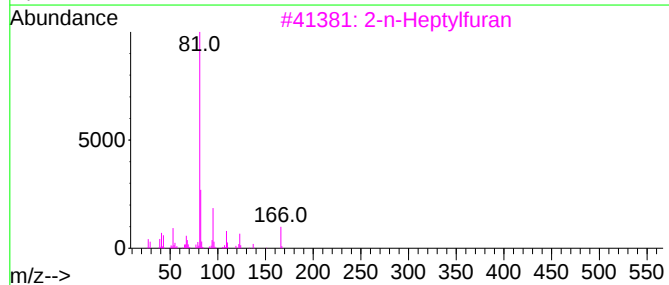
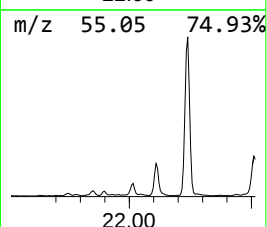
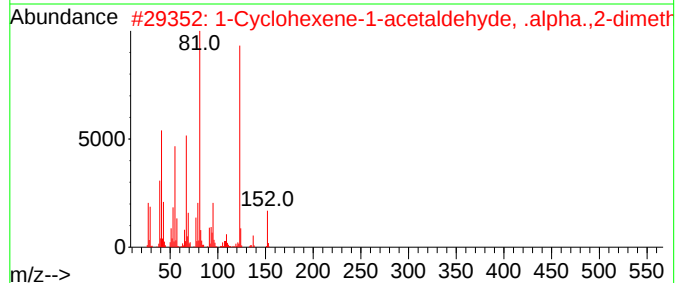
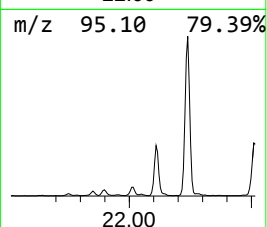
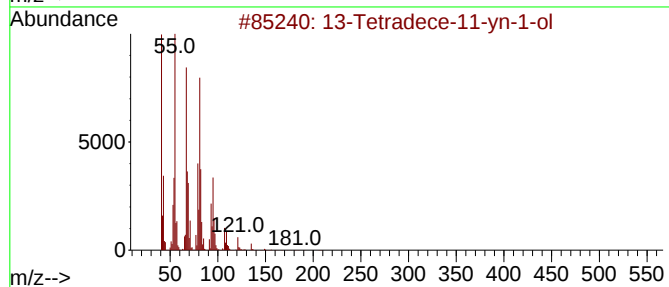
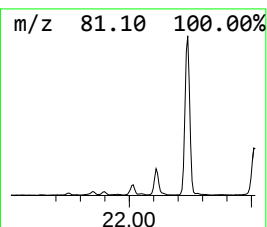
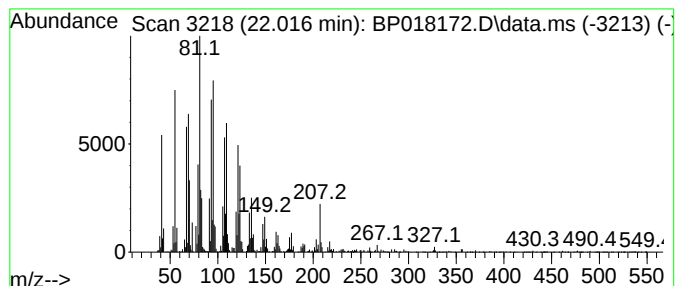
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 13-Tetradec-11-yn-1-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.016	4.45 ng/ul	266848	Chrysene-d12	21.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Tetradec-11-yn-1-ol	208	C14H24O	1000131-00-4	72
2			1-Cyclohexene-1-acetaldehyde, .a...	152	C10H16O	053155-80-9	27
3			2-n-Heptylfuran	166	C11H18O	003777-71-7	22
4			1-Cyclohexyl-1-pentyne	150	C11H18	067886-53-7	22
5			1-Naphthalenepropanol, .alpha.-e...	292	C19H32O2	055649-42-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
Data File : BP018172.D
Acq On : 15 Nov 2023 00:37
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Sample : 05158-01
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ClientSampleId :
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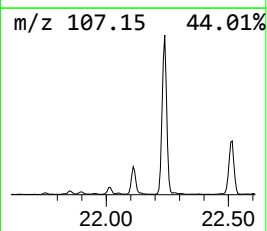
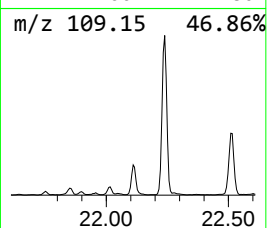
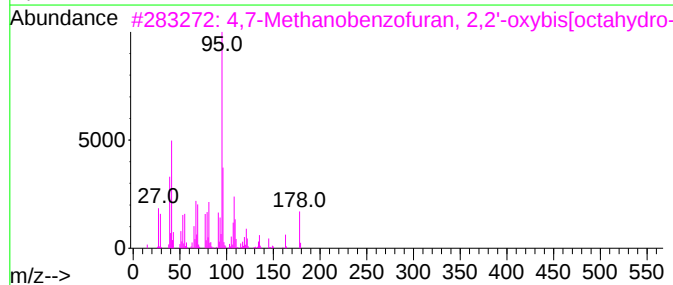
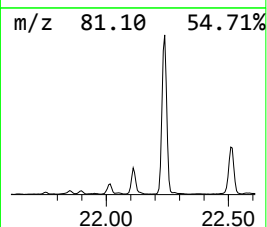
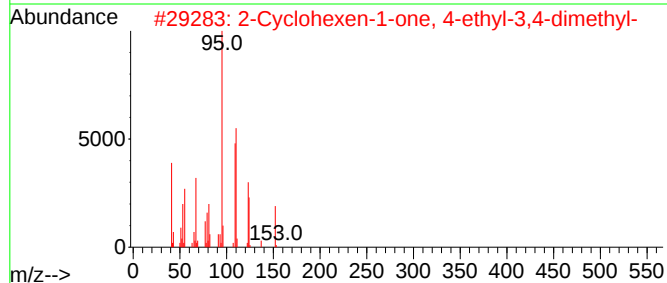
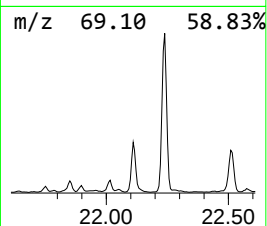
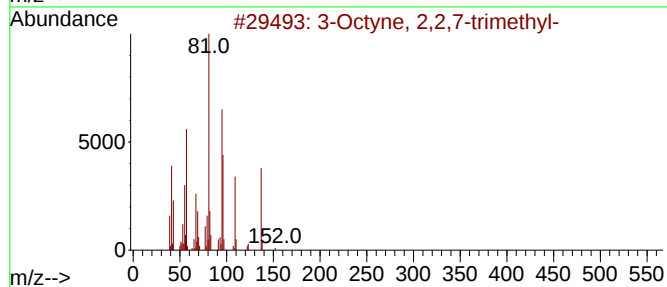
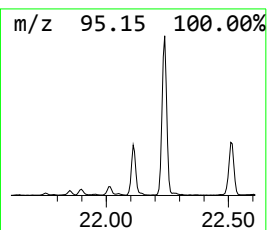
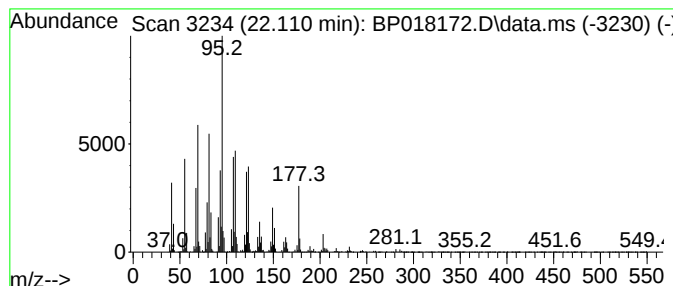
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.110	14.52 ng/ul	870665	Chrysene-d12	21.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	35
2			2-Cyclohexen-1-one, 4-ethyl-3,4-dimethyl-	152	C10H16O	017622-46-7	32
3			4,7-Methanobenzofuran, 2,2'-oxybis[octahydro-2H-benz[1,2-b:4,5-b']dipyrrolo[3,2-d:2',3'-d']pyrazine]	374	C24H38O3	087248-50-8	27
4			Cyclopentene, 1-isopropyl-2,3-dimethyl-	138	C10H18	007712-73-4	25
5			N-(1,1-Dimethylpropynyl)-2-furanmethanol	177	C10H11NO2	039108-97-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
Data File : BP018172.D
Acq On : 15 Nov 2023 00:37
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Sample : 05158-01
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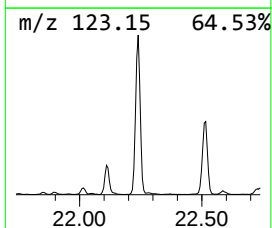
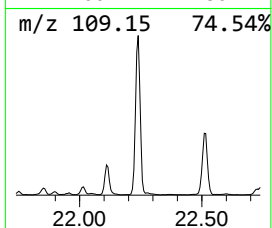
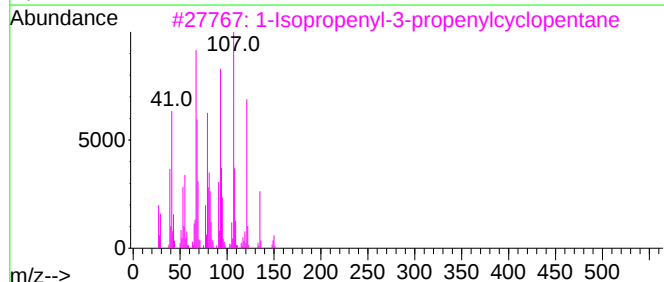
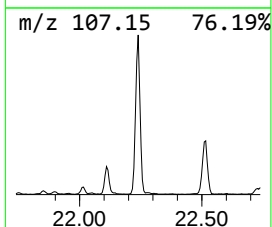
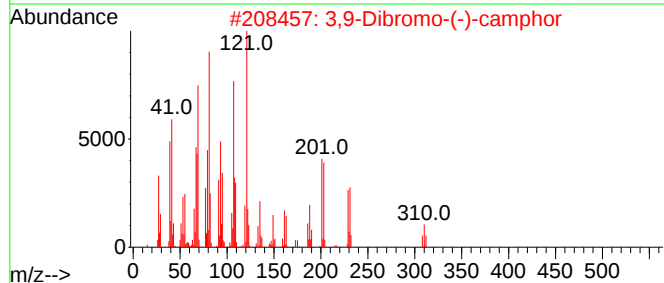
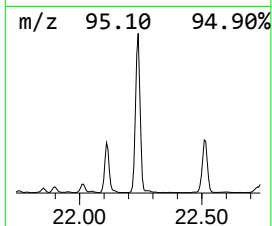
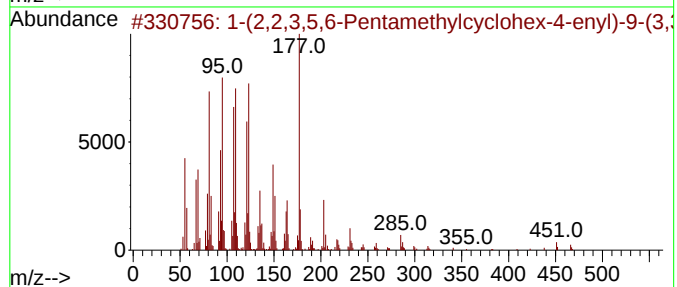
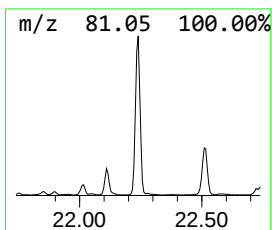
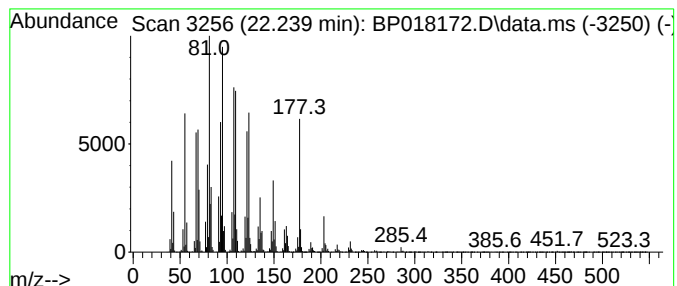
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-(2,2,3,5,6-Pentamethylcyc... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.239	79.10 ng/ul	4742860	Chrysene-d12	21.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2,2,3,5,6-Pentamethylcyclohex...	466	C34H58	1000373-94-7	90		
2	3,9-Dibromo-(-)-camphor	308	C10H14Br2O	064474-55-1	43		
3	1-Isopropenyl-3-propenylcyclopentane	150	C11H18	1000192-81-2	38		
4	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	35		
5	trans-Chrysanthanol	152	C10H16O	038043-83-3	30		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
Data File : BP018172.D
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Sample : 05158-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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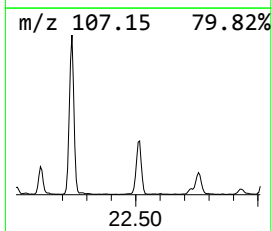
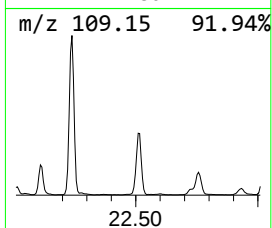
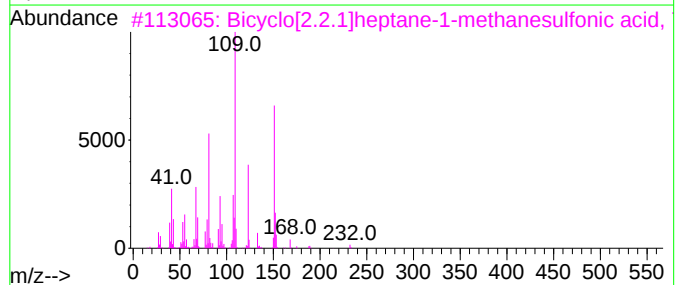
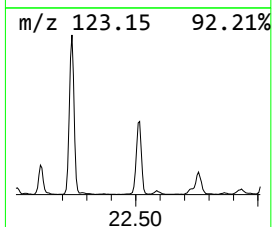
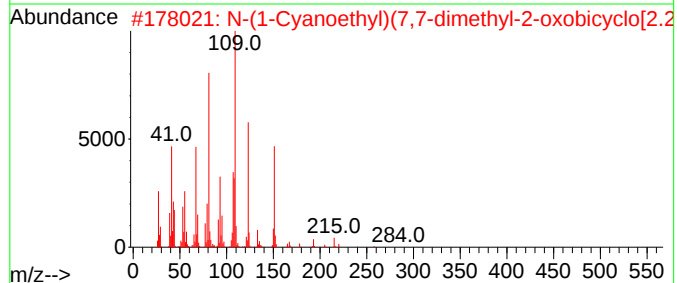
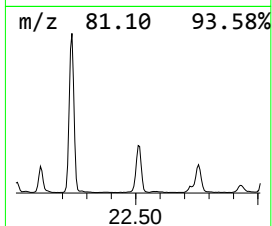
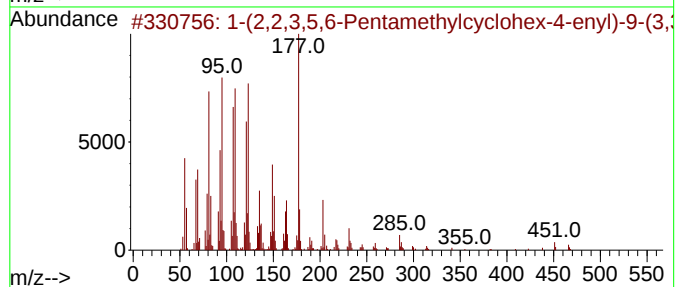
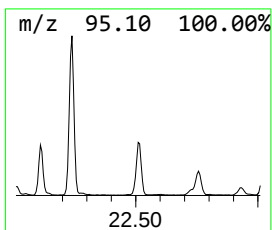
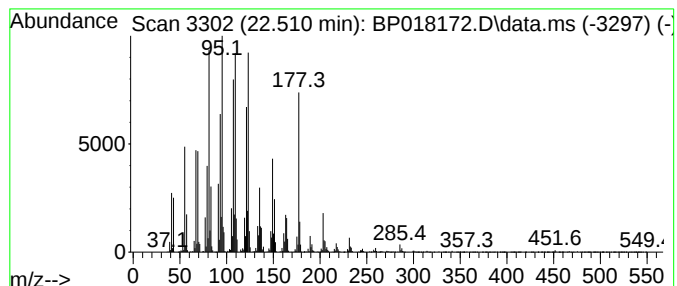
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.510	29.69 ng/ul	1780190	Chrysene-d12	21.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2,2,3,5,6-Pentamethylcyclohex...	466	C34H58	1000373-94-7	99
2			N-(1-Cyanoethyl)(7,7-dimethyl-2-...	284	C13H20N2O3S	1000194-50-3	30
3			Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	30
4			(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	22
5			2,3-DI-T-BUTYLCYCLOPROP-2-ENONE	166	C11H18O	019985-79-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
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ClientSampleId :
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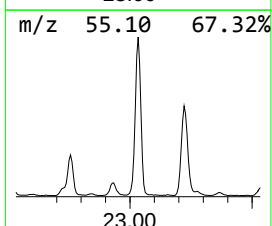
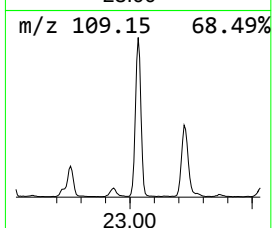
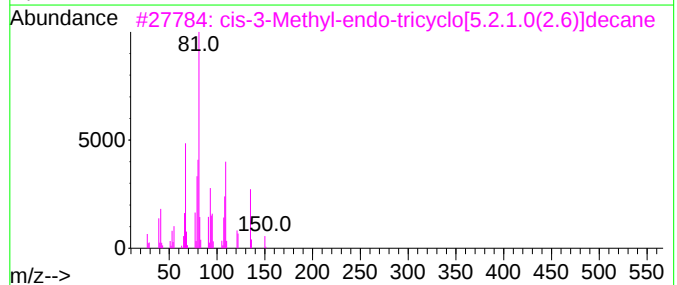
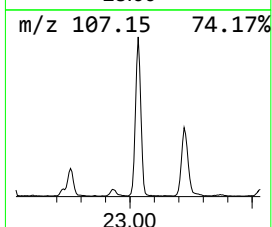
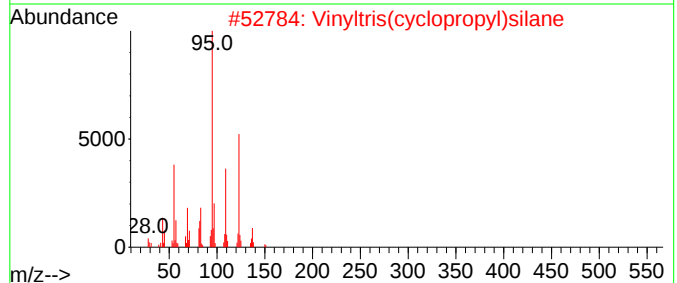
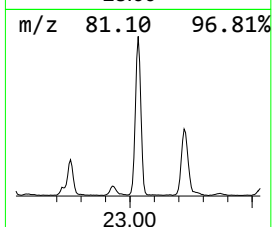
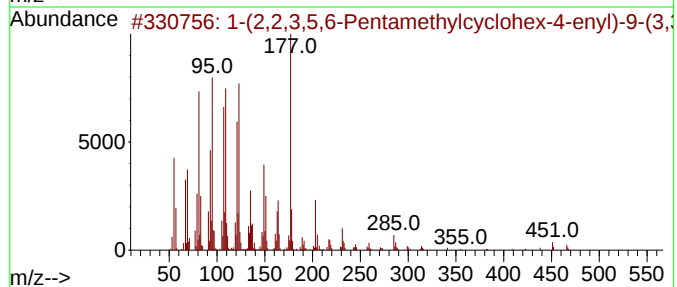
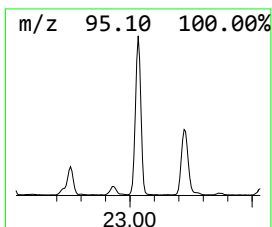
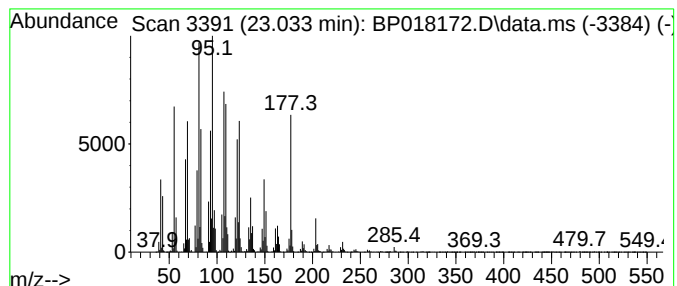
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 unknown-04 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.033	64.53 ng/ul	4463370	Perylene-d12	23.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2,2,3,5,6-Pentamethylcyclohex...	466	C34H58	1000373-94-7	91
2			Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	22
3			cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	22
4			trans-Chrysanthanol	152	C10H16O	038043-83-3	18
5			Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
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Sample : 05158-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

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ClientSampleId :
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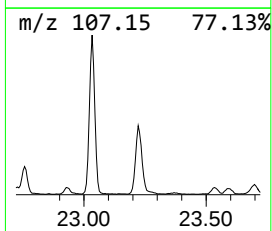
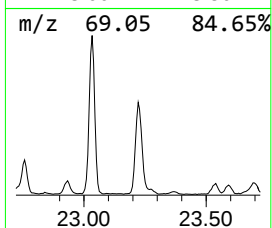
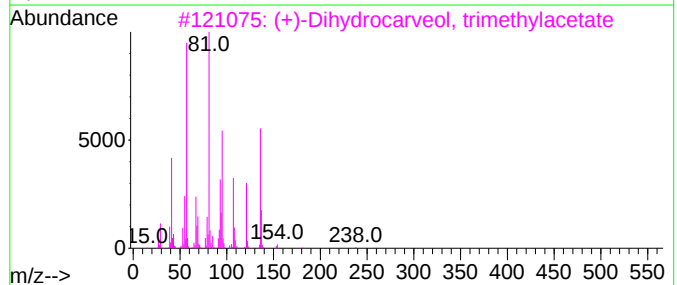
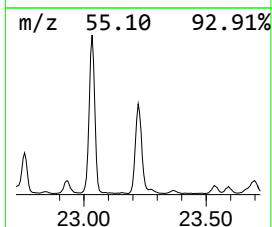
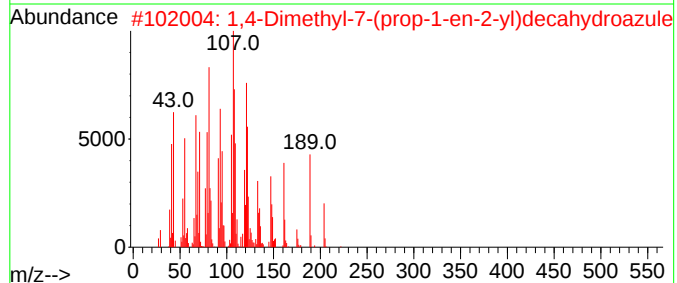
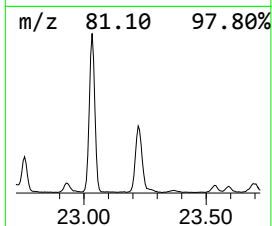
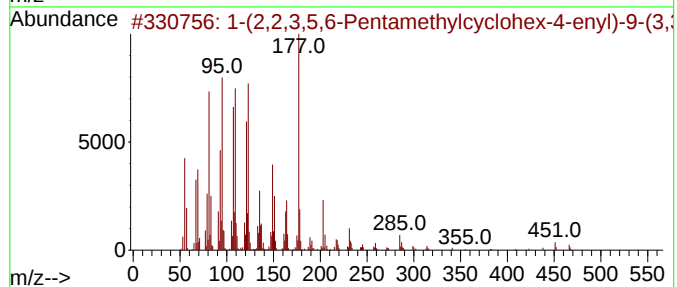
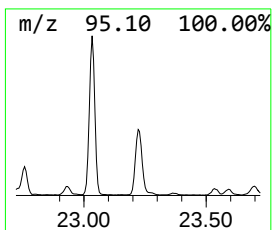
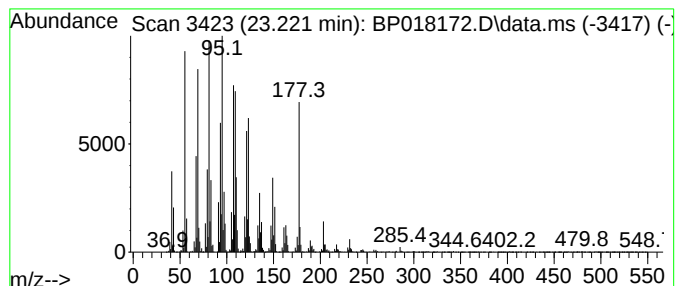
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 unknown-05 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.221	34.53 ng/ul	2388320	Perylene-d12	23.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2,2,3,5,6-Pentamethylcyclohex...	466	C34H58	1000373-94-7	87		
2	1,4-Dimethyl-7-(prop-1-en-2-yl)d...	222	C15H26O	021698-41-9	30		
3	(+)-Dihydrocarveol, trimethylace...	238	C15H26O2	1000462-97-7	20		
4	Cholestan-3-ol, 2-methylene-, (3...	400	C28H48O	022599-96-8	18		
5	Sesquirosefuran	218	C15H22O	039007-93-7	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
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Misc :
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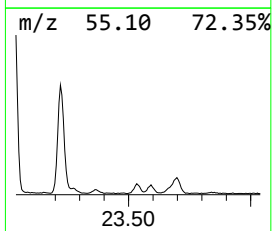
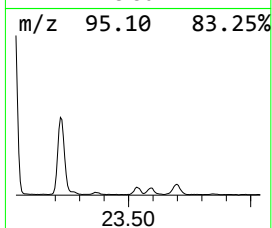
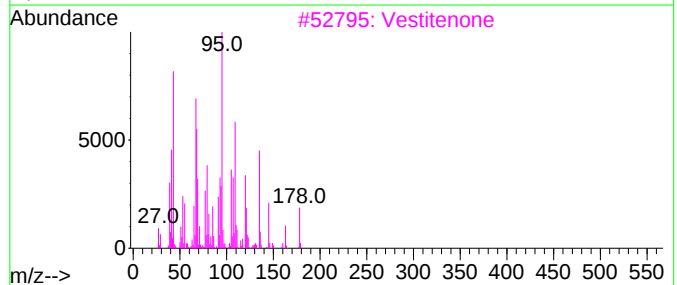
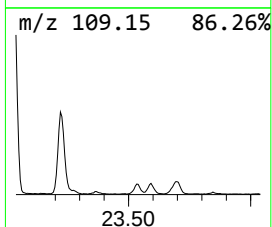
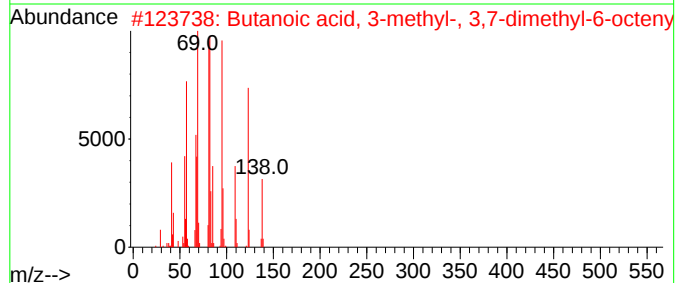
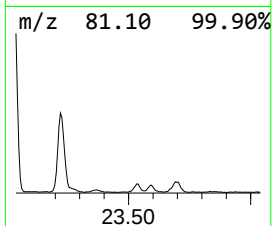
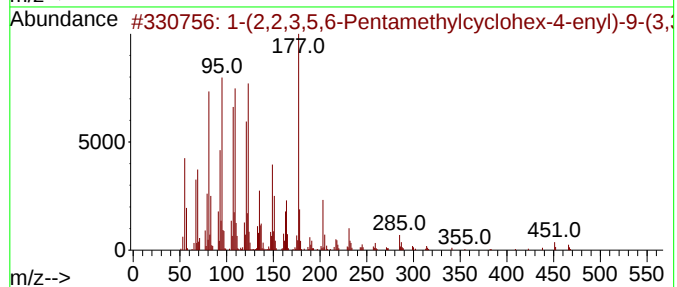
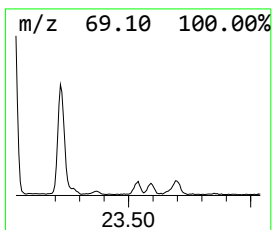
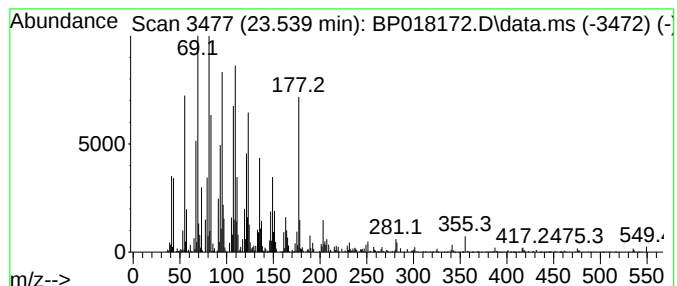
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 13 unknown-06 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.539	2.91 ng/ul	201082	Perylene-d12	23.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2,2,3,5,6-Pentamethylcyclohex...	466	C34H58	1000373-94-7	64
2			Butanoic acid, 3-methyl-, 3,7-di...	240	C15H28O2	068922-10-1	47
3			Vestitenone	178	C12H18O	069401-36-1	38
4			6-Methyl-6,7-dihydro-9H-5-oxa-9-...	177	C10H11NO2	1000210-20-2	38
5			(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111423\
 Data File : BP018172.D
 Acq On : 15 Nov 2023 00:37
 Operator : MA/JU
 Sample : 05158-01
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BH362

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
 Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentasilox...	9.163	2.2	ng/ul	49171	1	7.787	447493	20.0
n-Hexadecanoic ...	18.098	2.3	ng/ul	112691	4	17.245	997633	20.0
1,6,10-Dodecatr...	18.586	2.9	ng/ul	142816	4	17.245	997633	20.0
(DEL) Alkane: S...	21.039	4.2	ng/ul	248779	5	21.375	1199140	20.0
13-Tetradecene-11...	22.016	4.5	ng/ul	266848	5	21.375	1199140	20.0
unknown-01	22.110	14.5	ng/ul	870665	5	21.375	1199140	20.0
1-(2,2,3,5,6-Pe...	22.239	79.1	ng/ul	4742860	5	21.375	1199140	20.0
unknown-02	22.510	29.7	ng/ul	1780190	5	21.375	1199140	20.0
unknown-03	22.757	15.5	ng/ul	1071360	6	23.845	1383360	20.0
2-Methyl-3-(3-m...	22.933	3.9	ng/ul	270387	6	23.845	1383360	20.0
unknown-04	23.033	64.5	ng/ul	4463370	6	23.845	1383360	20.0
unknown-05	23.221	34.5	ng/ul	2388320	6	23.845	1383360	20.0
unknown-06	23.539	2.9	ng/ul	201082	6	23.845	1383360	20.0
(2Z,4E)-3,7,11-...	23.592	2.8	ng/ul	191954	6	23.845	1383360	20.0