

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
 Data File : BP013304.D
 Acq On : 24 Dec 2022 17:31
 Operator : CG/JU
 Sample : N6016-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DBYD5

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-BP120722.M
 Title : SVOA CALIBRATION

Signal : TIC: BP013304.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.246	7	10	12	rVB3	24746	25583	0.12%	0.013%
2	3.328	20	24	36	rVB	199568	278641	1.34%	0.144%
3	3.758	93	97	111	rBV	2183565	3131163	15.01%	1.615%
4	3.864	111	115	124	rVV	211818	281332	1.35%	0.145%
5	3.940	125	128	130	rVV	32299	36036	0.17%	0.019%
6	3.987	133	136	140	rVB2	21055	29772	0.14%	0.015%
7	4.087	149	153	158	rVB	56223	75217	0.36%	0.039%
8	4.458	213	216	221	rVB7	16024	28837	0.14%	0.015%
9	4.652	245	249	253	rVB3	32907	47763	0.23%	0.025%
10	5.034	308	314	321	rVB2	61902	103506	0.50%	0.053%
11	5.116	324	328	334	rBV2	38898	60519	0.29%	0.031%
12	5.263	347	353	358	rBV	25558	49741	0.24%	0.026%
13	6.528	564	568	575	rVB2	17582	32542	0.16%	0.017%
14	7.105	658	666	679	rBV	2731536	4324362	20.72%	2.231%
15	7.269	684	694	703	rBV	2332605	3597160	17.24%	1.856%
16	7.369	708	711	718	rVV3	17909	34425	0.16%	0.018%
17	7.469	721	728	737	rVV	2920593	4554569	21.83%	2.350%
18	7.552	738	742	751	rVV3	23029	55025	0.26%	0.028%
19	7.940	800	808	815	rBV	2147784	3281172	15.72%	1.693%
20	8.005	815	819	825	rVB4	15292	27934	0.13%	0.014%
21	8.075	825	831	837	rBV	98817	153994	0.74%	0.079%
22	8.652	922	929	941	rVV	2599286	4164917	19.96%	2.149%
23	9.110	999	1007	1016	rBV	2637056	4278313	20.50%	2.207%
24	9.263	1028	1033	1038	rVB7	24753	39823	0.19%	0.021%
25	9.504	1066	1074	1080	rBV	59264	98630	0.47%	0.051%
26	9.704	1102	1108	1112	rVB3	10622	21464	0.10%	0.011%
27	9.834	1119	1130	1148	rBV	2213433	3641529	17.45%	1.879%
28	10.051	1163	1167	1174	rVB8	14033	26273	0.13%	0.014%
29	10.375	1214	1222	1243	rBV	3114178	5243387	25.13%	2.705%
30	10.751	1278	1286	1294	rBV	2516056	4246943	20.35%	2.191%
31	10.893	1302	1310	1328	rBV	2043415	3661355	17.55%	1.889%
32	11.134	1344	1351	1361	rVV	133935	223995	1.07%	0.116%
33	11.222	1361	1366	1372	rVB	82097	129632	0.62%	0.067%
34	11.281	1372	1376	1381	rBV8	16145	25039	0.12%	0.013%
35	11.540	1416	1420	1427	rBV9	12044	27704	0.13%	0.014%
36	12.157	1522	1525	1530	rBV5	16006	23811	0.11%	0.012%

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37	12.245	1535	1540	1541	rBV2	19626	29596	0.14%	0.015%
38	12.275	1541	1545	1551	rVV	33819	58626	0.28%	0.030%
39	12.340	1551	1556	1561	rVV	53845	81412	0.39%	0.042%
40	12.851	1637	1643	1648	rBV10	10725	22133	0.11%	0.011%
41	13.398	1729	1736	1741	rVB3	46617	80000	0.38%	0.041%
42	13.510	1751	1755	1757	rBV4	17566	25113	0.12%	0.013%
43	13.575	1760	1766	1772	rVB	496211	686831	3.29%	0.354%
44	13.769	1793	1799	1802	rBV6	13482	25361	0.12%	0.013%
45	13.992	1829	1837	1846	rBV	4559688	6394238	30.64%	3.299%
46	14.104	1853	1856	1862	rVB8	14395	22763	0.11%	0.012%
47	14.281	1879	1886	1897	rBV	5635155	8152109	39.07%	4.206%
48	14.469	1915	1918	1922	rVB	36023	48780	0.23%	0.025%
49	14.587	1931	1938	1946	rVB	3294161	4863899	23.31%	2.509%
50	14.787	1961	1972	1989	rBV	1918077	3162682	15.16%	1.632%
51	14.939	1993	1998	2002	rVV2	69262	113532	0.54%	0.059%
52	14.986	2003	2006	2013	rVB5	55928	87959	0.42%	0.045%
53	15.251	2047	2051	2057	rVB9	16153	25359	0.12%	0.013%
54	15.581	2100	2107	2113	rBV	7093841	9850387	47.21%	5.082%
55	15.634	2113	2116	2121	rVB	53791	76048	0.36%	0.039%
56	15.698	2121	2127	2135	rBV	1712404	2315206	11.10%	1.194%
57	15.822	2144	2148	2154	rVB	35075	56909	0.27%	0.029%
58	15.945	2164	2169	2175	rVB	350553	472566	2.26%	0.244%
59	16.139	2199	2202	2210	rVB10	23448	39411	0.19%	0.020%
60	16.210	2210	2214	2219	rBV2	94828	121079	0.58%	0.062%
61	16.292	2224	2228	2233	rVB8	22284	39786	0.19%	0.021%
62	16.445	2249	2254	2261	rBV10	16477	39224	0.19%	0.020%
63	16.516	2262	2266	2269	rVV3	29104	35229	0.17%	0.018%
64	16.728	2298	2302	2307	rBV4	45554	58864	0.28%	0.030%
65	17.222	2381	2386	2389	rBV5	36279	55646	0.27%	0.029%
66	17.345	2400	2407	2417	rBV	4198716	6228498	29.85%	3.213%
67	17.445	2417	2424	2432	rVV	7113986	10011965	47.98%	5.165%
68	17.551	2439	2442	2449	rVB5	49743	69795	0.33%	0.036%
69	17.698	2463	2467	2477	rBV8	90287	158684	0.76%	0.082%
70	17.998	2515	2518	2523	rVB6	42175	49349	0.24%	0.025%
71	18.098	2532	2535	2541	rVB6	42066	69505	0.33%	0.036%
72	18.157	2541	2545	2550	rBV	118502	169887	0.81%	0.088%
73	18.216	2550	2555	2565	rBV	1874362	2586415	12.40%	1.334%
74	18.339	2574	2576	2581	rVB5	43422	54641	0.26%	0.028%
75	18.410	2584	2588	2592	rVB	145647	195186	0.94%	0.101%
76	18.463	2594	2597	2601	rBV2	77915	88544	0.42%	0.046%

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77	18.551	2607	2612	2618	rBV3	230265	370304	1.77%	0.191%
78	18.627	2621	2625	2629	rBV	151423	179051	0.86%	0.092%
79	18.698	2634	2637	2640	rBV2	66456	93400	0.45%	0.048%
80	18.780	2647	2651	2656	rBV	212564	262068	1.26%	0.135%
81	19.116	2705	2708	2712	rVB2	129049	164690	0.79%	0.085%
82	19.251	2728	2731	2735	rBV	99180	120625	0.58%	0.062%
83	19.327	2738	2744	2747	rBV3	287179	614754	2.95%	0.317%
84	19.445	2760	2764	2773	rBV	603458	854659	4.10%	0.441%
85	19.680	2798	2804	2814	rVB	10419408	14162016	67.87%	7.306%
86	19.827	2824	2829	2836	rBV	2765388	3344825	16.03%	1.726%
87	20.169	2883	2887	2893	rBV3	422818	692609	3.32%	0.357%
88	21.127	3045	3050	3055	rBV	2291902	3776154	18.10%	1.948%
89	21.433	3097	3102	3107	rBV	5693214	7761921	37.20%	4.004%
90	23.757	3490	3497	3514	rVB2	7794058	16008280	76.72%	8.259%
91	23.915	3517	3524	3535	rVB2	3891304	8010447	38.39%	4.133%
92	24.527	3624	3628	3638	rVB	1177863	2387262	11.44%	1.232%
93	26.445	3947	3954	3975	rVB2	2029118	7043683	33.76%	3.634%
94	28.498	4295	4303	4329	rVB3	5353739	20866527	100.00%	10.765%
95	29.009	4383	4390	4400	rVB6	1356499	4333862	20.77%	2.236%

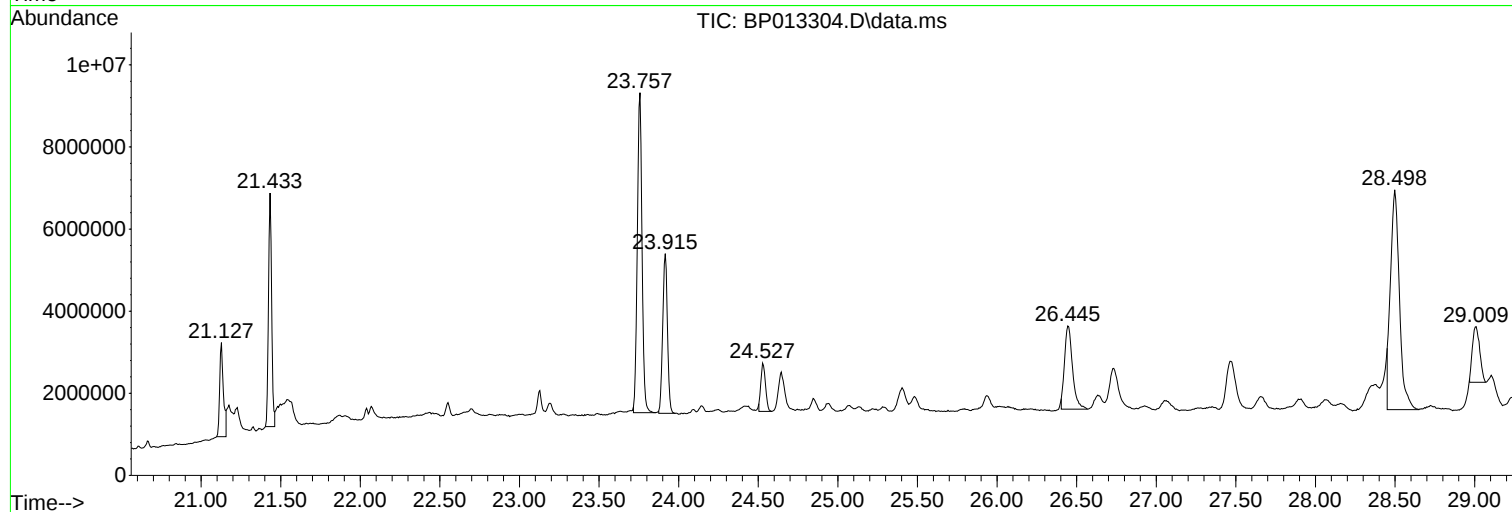
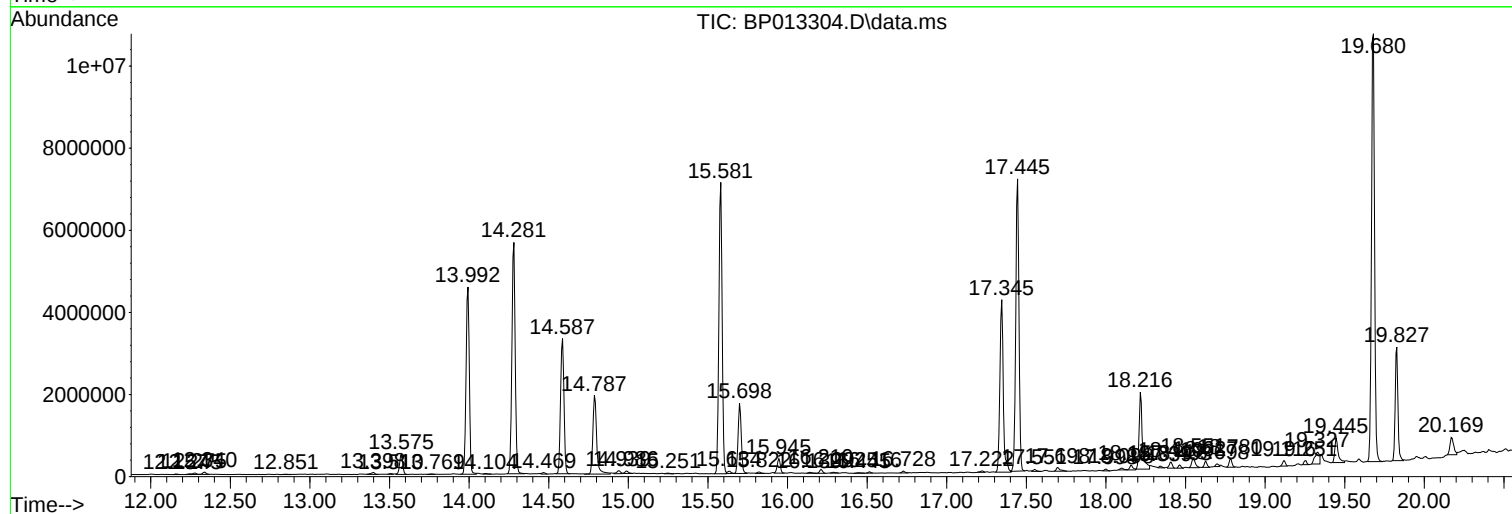
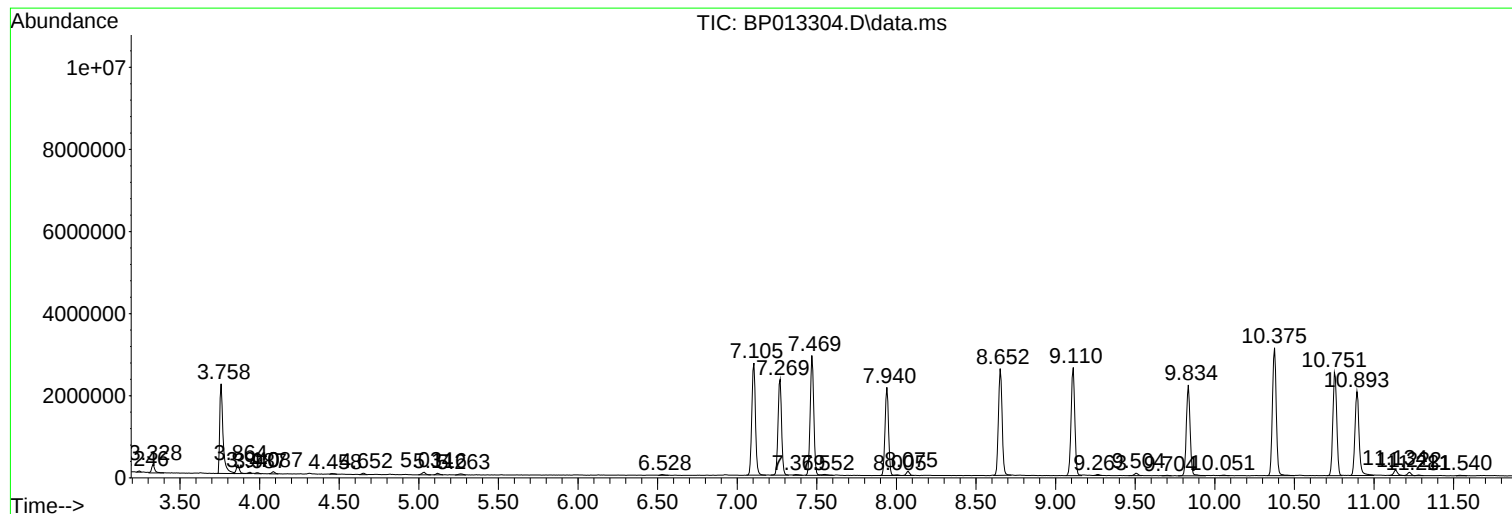
Sum of corrected areas: 193832462

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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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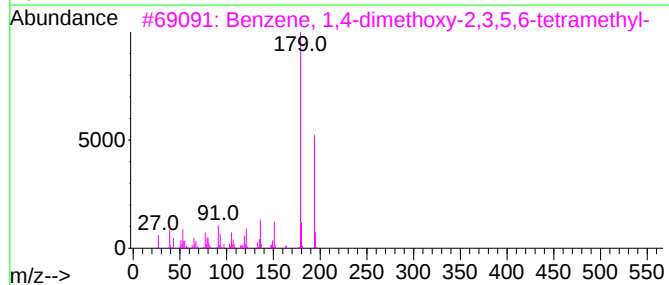
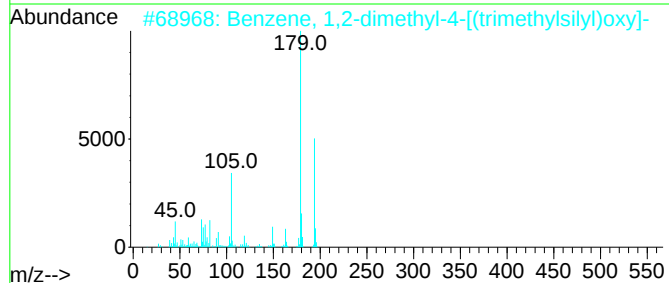
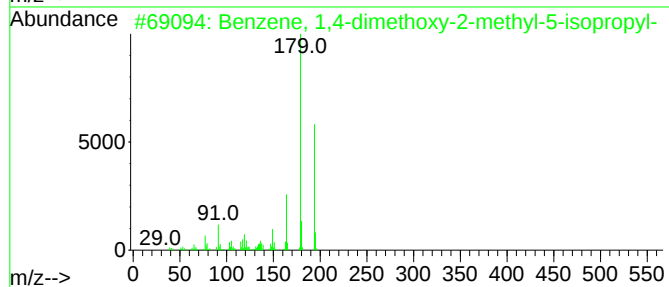
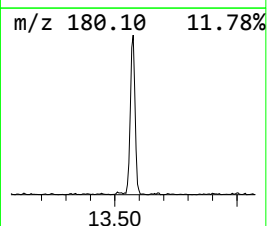
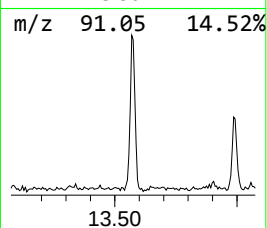
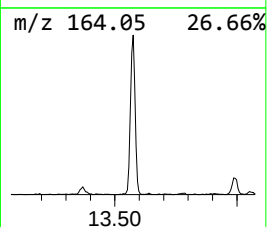
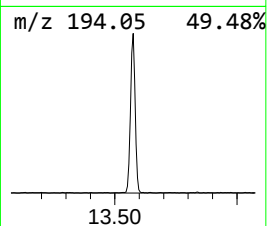
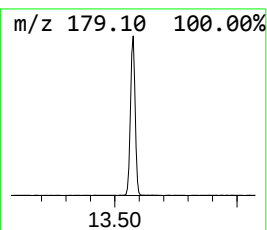
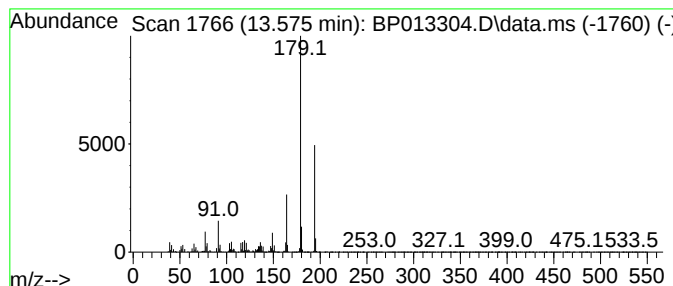
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzene, 1,4-dimethoxy-2-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.575	2.82 ng/ul	686831	Acenaphthene-d10	14.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-dimethoxy-2-methyl-...	194	C12H18O2	014753-08-3	98
2			Benzene, 1,2-dimethyl-4-[(trimet...	194	C11H18OSi	017994-04-6	74
3			Benzene, 1,4-dimethoxy-2,3,5,6-t...	194	C12H18O2	013199-54-7	72
4			3-Hydroxybenzaldehyde, trimethyl...	194	C10H14O2Si	001012-30-2	72
5			5-Acetoacenaphthylene	194	C14H10O	068399-52-0	64



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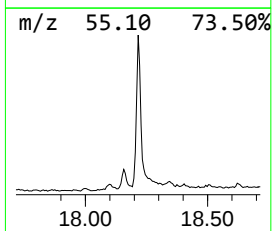
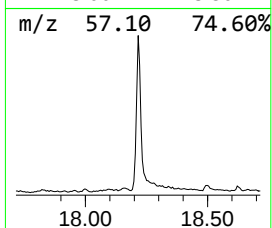
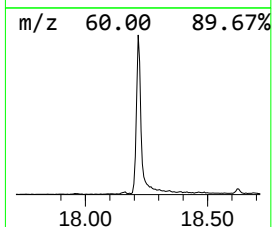
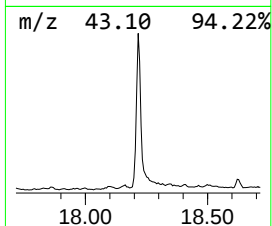
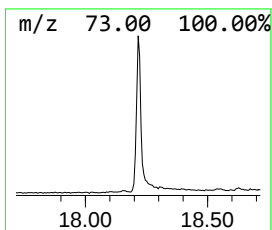
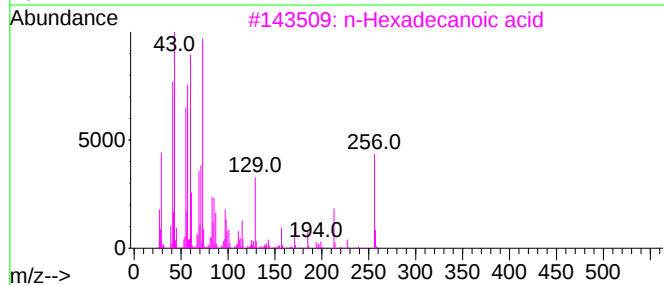
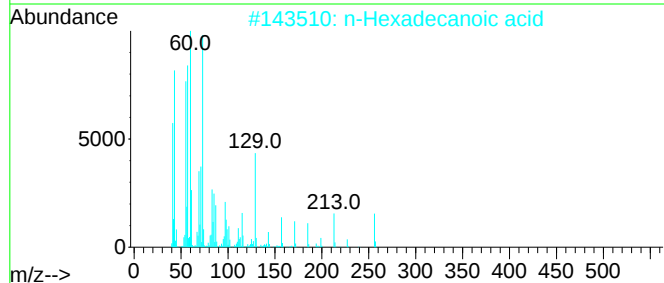
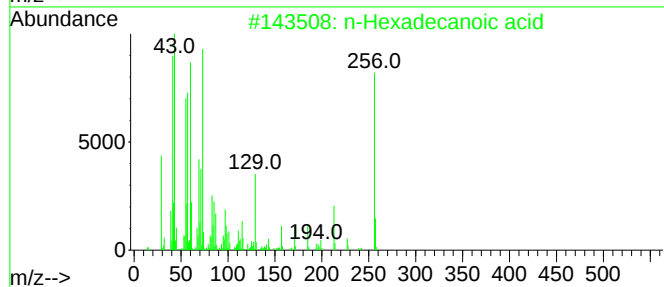
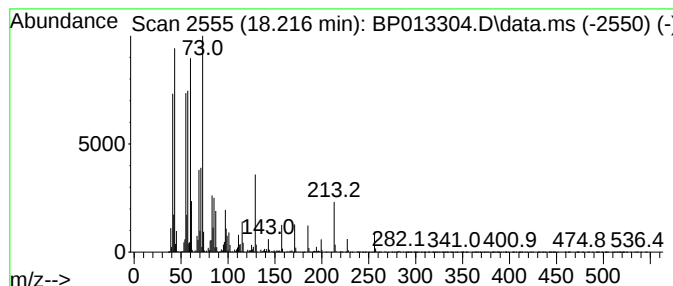
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	8.31 ng/ul	2586420	Phenanthrene-d10	17.345

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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5			Tridecanoic acid	214	C13H26O2	000638-53-9	95



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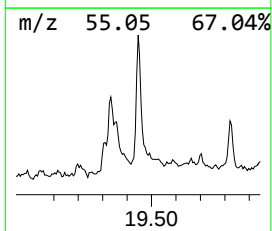
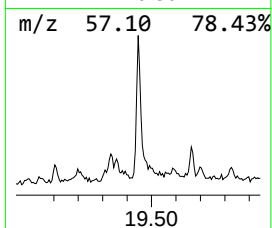
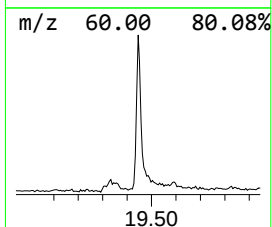
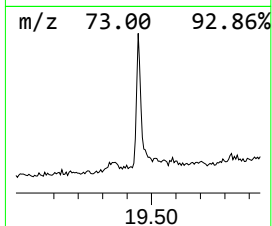
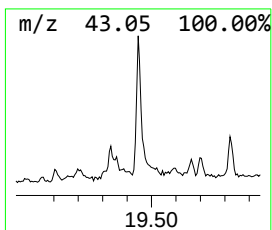
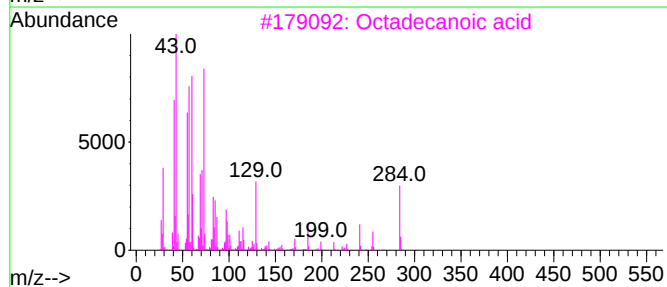
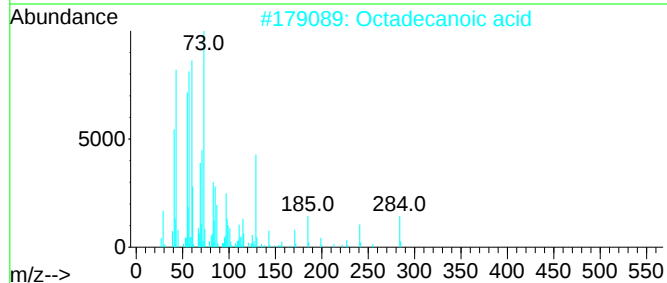
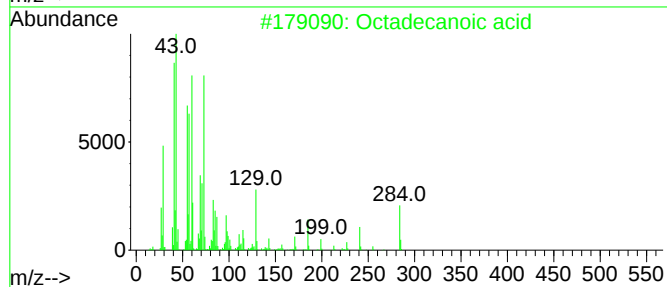
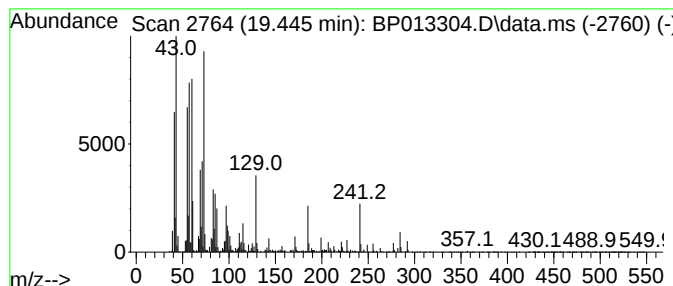
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	2.20 ng/ul	854659	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013304.D
Acq On : 24 Dec 2022 17:31
Operator : CG/JU
Sample : N6016-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD5

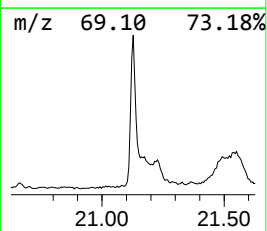
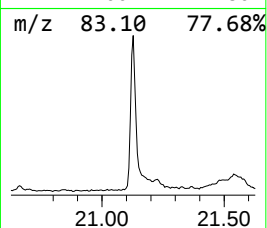
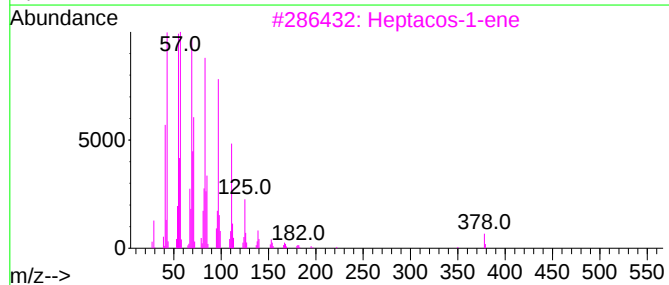
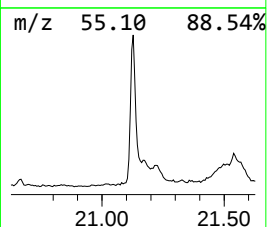
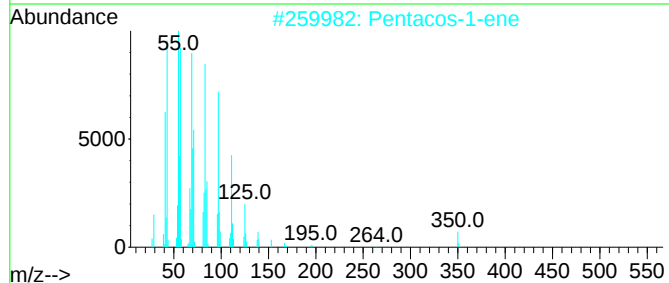
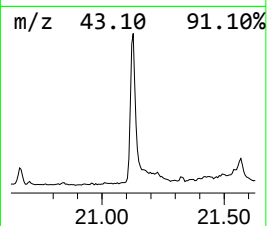
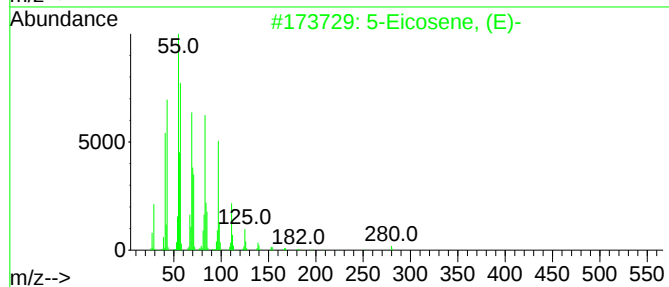
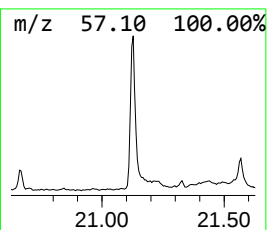
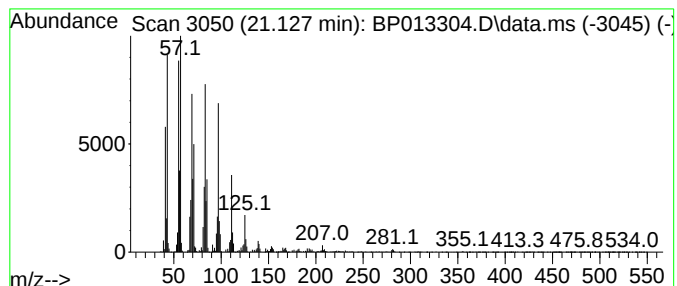
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	9.73 ng/ul	3776150	Chrysene-d12	21.433

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	96
2	Pentacos-1-ene		350	C25H50	016980-85-1	94
3	Heptacos-1-ene		378	C27H54	015306-27-1	94
4	1-Heneicosanol		312	C21H44O	015594-90-8	93
5	Octacosanol		410	C28H58O	000557-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013304.D
Acq On : 24 Dec 2022 17:31
Operator : CG/JU
Sample : N6016-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD5

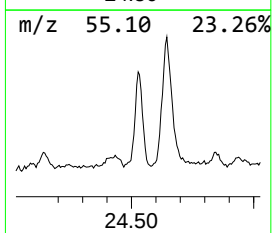
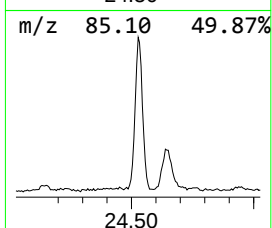
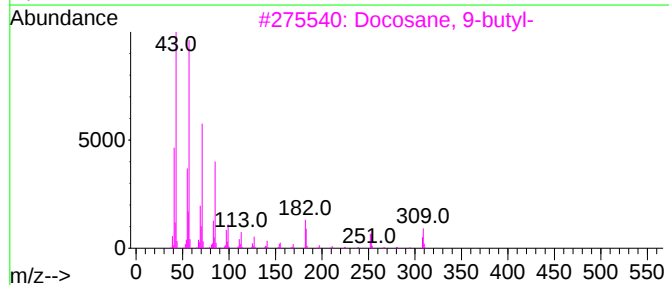
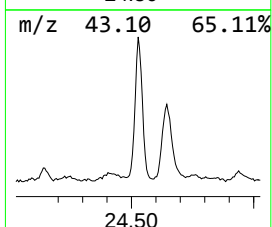
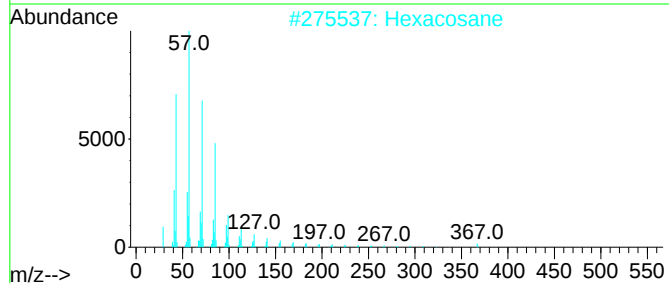
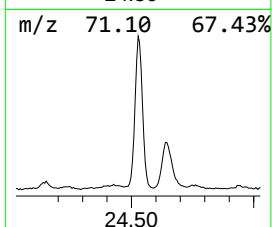
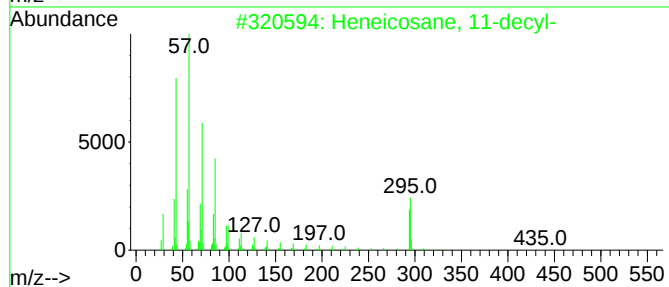
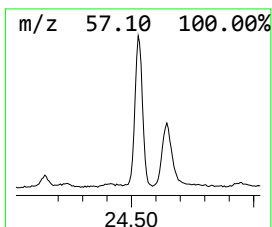
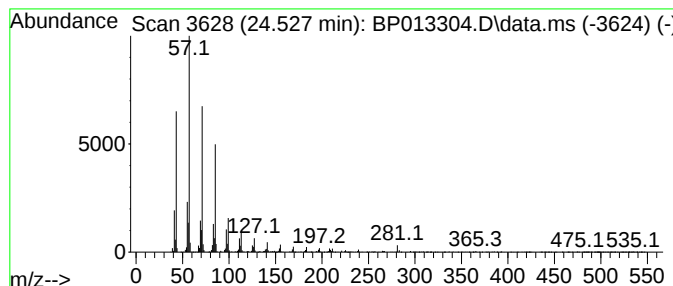
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.527	5.96 ng/ul	2387260	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	98
2			Hexacosane	366	C26H54	000630-01-3	93
3			Docosane, 9-butyl-	366	C26H54	055282-14-9	93
4			2-Methyltetracosane	352	C25H52	001560-78-7	93
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013304.D
Acq On : 24 Dec 2022 17:31
Operator : CG/JU
Sample : N6016-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD5

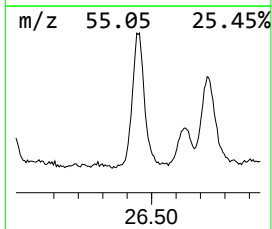
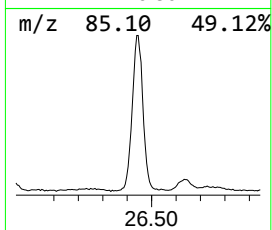
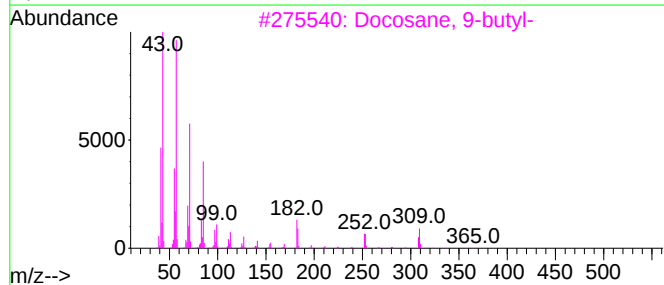
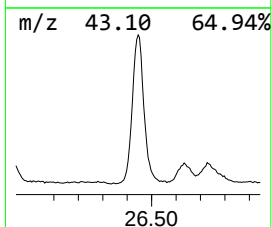
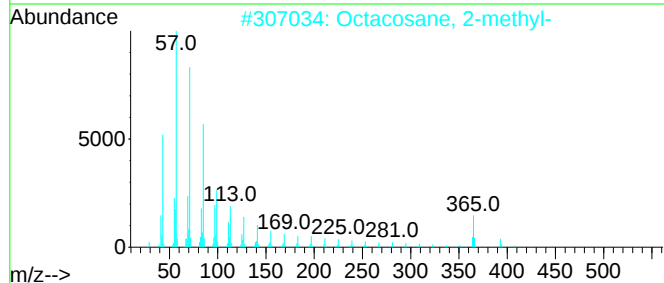
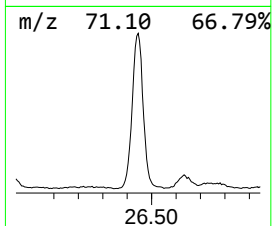
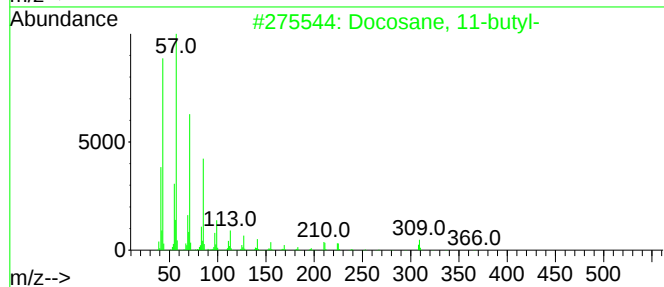
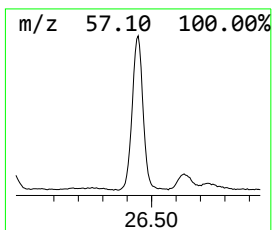
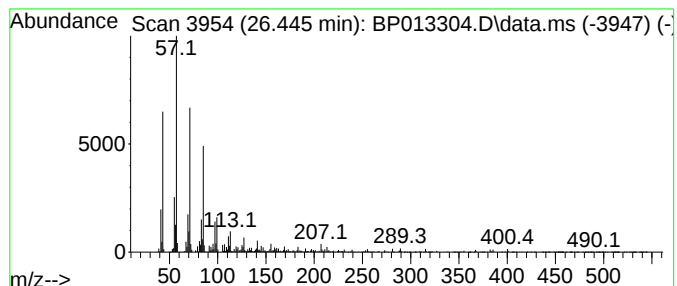
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.445	17.59 ng/ul	7043680	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	93
3			Docosane, 9-butyl-	366	C26H54	055282-14-9	93
4			Heptacosane	380	C27H56	000593-49-7	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013304.D
Acq On : 24 Dec 2022 17:31
Operator : CG/JU
Sample : N6016-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD5

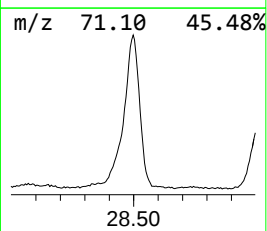
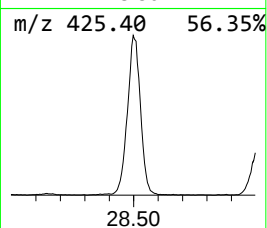
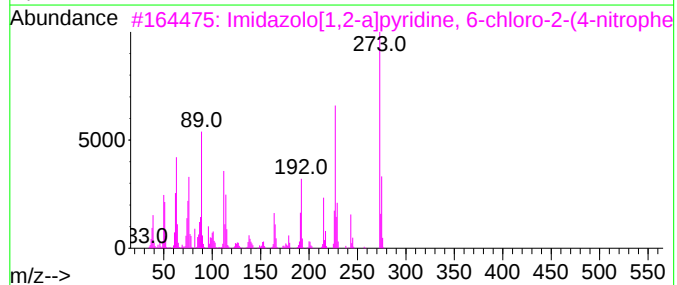
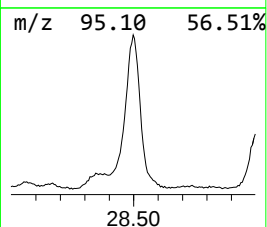
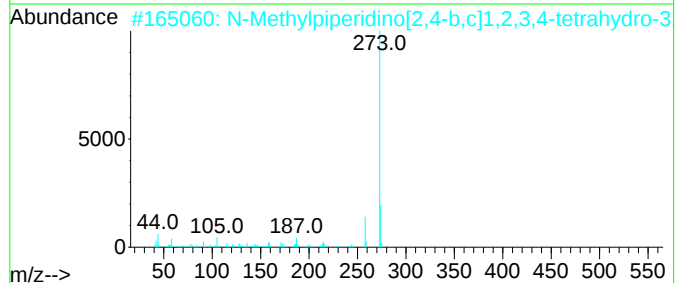
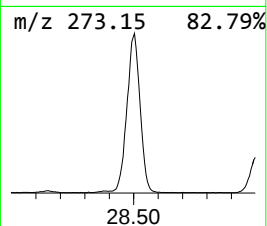
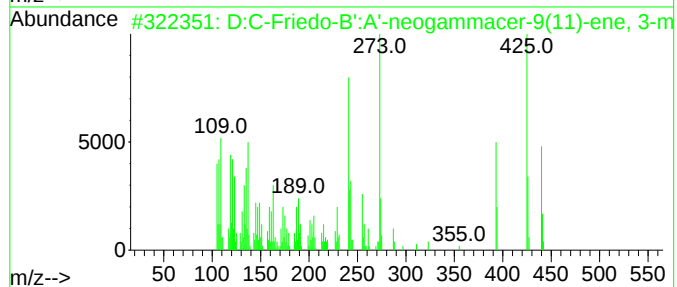
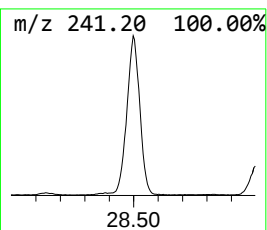
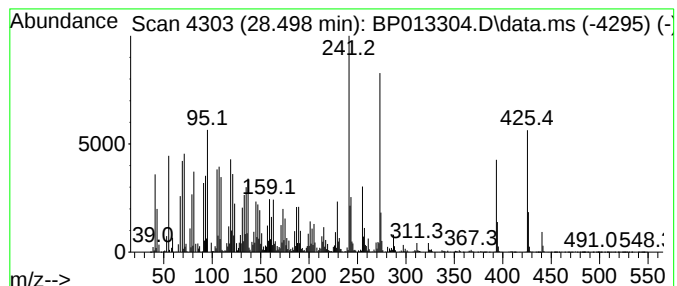
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.497	52.10 ng/ul	20866500	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	58
2			N-Methylpiperidino[2,4-b,c]1,2,3...	273	C18H27NO	1000128-54-7	25
3			Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	25
4			Lupeol	426	C30H50O	000545-47-1	15
5			6-(Trifluoromethoxy)-1H-indole-2...	273	C12H10F3NO3	1000499-75-7	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013304.D
Acq On : 24 Dec 2022 17:31
Operator : CG/JU
Sample : N6016-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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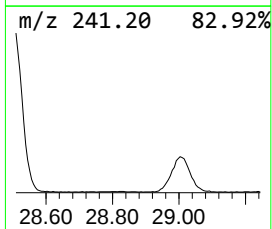
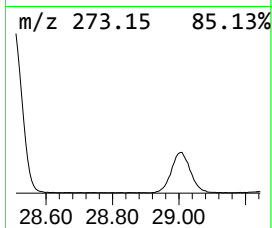
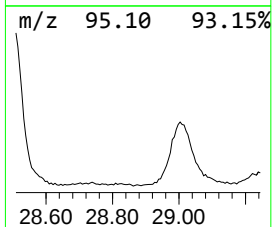
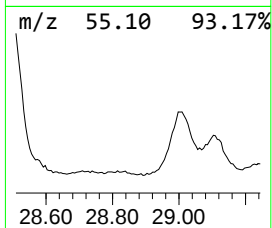
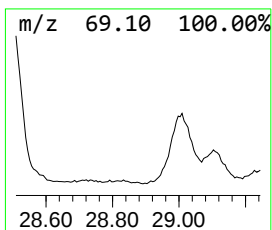
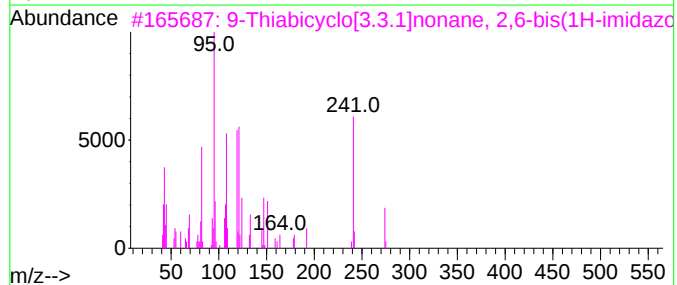
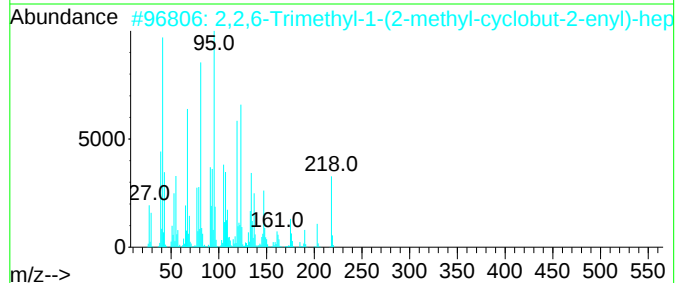
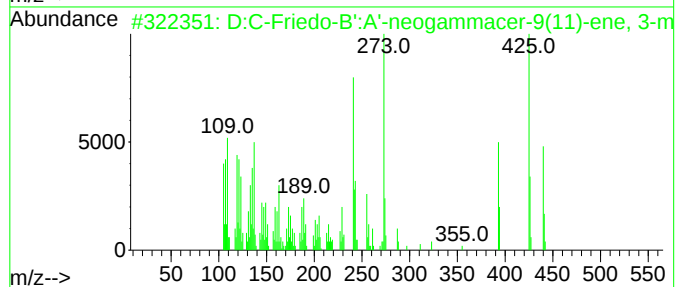
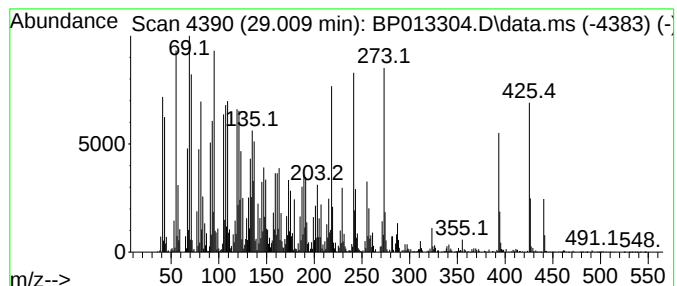
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.009	10.82 ng/ul	4333860	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	64
2			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38
3			9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	30
4			(3S,5R,8S)-3,8-Dimethyl-5-(prop-...	218	C15H22O	018374-76-0	25
5			7-Isopropenyl-1,4a-dimethyl-4,4a...	218	C15H22O	000473-08-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013304.D
Acq On : 24 Dec 2022 17:31
Operator : CG/JU
Sample : N6016-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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
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n-Hexadecanoic ...	18.216	8.3	ng/ul	2586420	4	17.345	6228500	20.0
Octadecanoic acid	19.445	2.2	ng/ul	854659	5	21.433	7761920	20.0
4-(3-Fluoro-8-n...	19.827	8.6	ng/ul	3344830	5	21.433	7761920	20.0
(DEL) Alkane: S...	21.127	9.7	ng/ul	3776150	5	21.433	7761920	20.0
(DEL) Alkane: S...	24.527	6.0	ng/ul	2387260	6	23.915	8010450	20.0
(DEL) Alkane: S...	26.445	17.6	ng/ul	7043680	6	23.915	8010450	20.0
D:C-Friedo-B':A...	28.497	52.1	ng/ul	20866500	6	23.915	8010450	20.0
unknown-01	29.009	10.8	ng/ul	4333860	6	23.915	8010450	20.0