

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
 Data File : BP013208.D
 Acq On : 21 Dec 2022 15:12
 Operator : CG/JU
 Sample : N6014-04
 Misc :
 ALS Vial : 90 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DBXR5

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: BP013208.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	21	25	35	rVB	129301	174605	1.11%	0.105%
2	3.764	94	98	113	rBV	1977171	2855824	18.17%	1.724%
3	4.093	150	154	163	rVB	57465	79648	0.51%	0.048%
4	5.040	312	315	322	rVB2	28529	45403	0.29%	0.027%
5	5.275	351	355	359	rBV4	11816	20164	0.13%	0.012%
6	6.928	632	636	642	rVB9	15192	26691	0.17%	0.016%
7	7.110	660	667	680	rVB	2508103	3954036	25.16%	2.387%
8	7.275	688	695	708	rVB	1916233	2925073	18.61%	1.766%
9	7.381	709	713	718	rVB7	16462	25953	0.17%	0.016%
10	7.475	722	729	742	rBV	2371017	3810037	24.25%	2.300%
11	7.952	803	810	817	rBV	1993189	3134690	19.95%	1.892%
12	8.022	817	822	829	rVB2	25115	47161	0.30%	0.028%
13	8.169	840	847	851	rBV10	11745	25406	0.16%	0.015%
14	8.657	920	930	944	rBV	3114239	5093873	32.42%	3.075%
15	9.116	1000	1008	1018	rBV	2426022	3886488	24.73%	2.346%
16	9.275	1031	1035	1041	rVB6	20518	34115	0.22%	0.021%
17	9.428	1055	1061	1066	rBV5	14721	28442	0.18%	0.017%
18	9.516	1070	1076	1086	rVB	33010	61897	0.39%	0.037%
19	9.710	1101	1109	1116	rBV	576666	894631	5.69%	0.540%
20	9.840	1123	1131	1141	rBV	2045284	3373540	21.47%	2.036%
21	10.069	1164	1170	1176	rVB	9110	20403	0.13%	0.012%
22	10.381	1216	1223	1236	rBV	3291565	5356289	34.09%	3.233%
23	10.663	1265	1271	1277	rBV3	10641	21079	0.13%	0.013%
24	10.763	1280	1288	1296	rBV	2704241	4443754	28.28%	2.682%
25	10.904	1300	1312	1326	rBV	2194824	3935117	25.04%	2.375%
26	11.169	1353	1357	1364	rVB10	11115	22281	0.14%	0.013%
27	11.428	1394	1401	1410	rBV7	15623	35945	0.23%	0.022%
28	11.957	1487	1491	1496	rVB5	12892	19314	0.12%	0.012%
29	12.175	1521	1528	1531	rBV6	11320	16761	0.11%	0.010%
30	12.345	1551	1557	1561	rBV2	58493	93451	0.59%	0.056%
31	12.392	1561	1565	1575	rVB	131293	199283	1.27%	0.120%
32	13.022	1668	1672	1677	rVB8	16099	23530	0.15%	0.014%
33	13.287	1707	1717	1719	rBV8	17652	35339	0.22%	0.021%
34	13.328	1720	1724	1728	rVV7	20970	34150	0.22%	0.021%
35	13.404	1734	1737	1741	rVB	26012	31159	0.20%	0.019%
36	13.463	1741	1747	1753	rBV	307335	423815	2.70%	0.256%

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37	13.545	1753	1761	1762	rBV8	8633	17992	0.11%	0.011%
38	13.704	1785	1788	1792	rVB6	14583	19747	0.13%	0.012%
39	13.916	1818	1824	1829	rBV6	29325	56329	0.36%	0.034%
40	13.998	1831	1838	1847	rBV	5268511	7104757	45.21%	4.288%
41	14.139	1854	1862	1867	rBV	232781	349381	2.22%	0.211%
42	14.192	1867	1871	1875	rVB7	33270	43382	0.28%	0.026%
43	14.286	1880	1887	1895	rBV	6232257	8890456	56.58%	5.366%
44	14.428	1906	1911	1916	rVB2	56447	77136	0.49%	0.047%
45	14.481	1916	1920	1925	rVB3	31271	45743	0.29%	0.028%
46	14.545	1926	1931	1933	rBV5	30012	42094	0.27%	0.025%
47	14.592	1933	1939	1945	rBV	3685184	5312083	33.80%	3.206%
48	14.651	1945	1949	1953	rBV	115517	148696	0.95%	0.090%
49	14.692	1954	1956	1966	rVB8	46421	79410	0.51%	0.048%
50	14.786	1966	1972	1986	rBV	1592280	2647048	16.85%	1.598%
51	14.898	1987	1991	1995	rBV4	65275	78078	0.50%	0.047%
52	14.951	1995	2000	2005	rBV6	84189	175078	1.11%	0.106%
53	15.263	2049	2053	2059	rVB9	16045	31302	0.20%	0.019%
54	15.369	2065	2071	2073	rBV7	10128	17928	0.11%	0.011%
55	15.486	2086	2091	2092	rBV4	28583	41156	0.26%	0.025%
56	15.586	2101	2108	2122	rBV	7373304	10504128	66.85%	6.340%
57	15.704	2122	2128	2136	rVV	1871759	2442538	15.54%	1.474%
58	15.828	2144	2149	2156	rVB2	41054	71588	0.46%	0.043%
59	15.951	2165	2170	2176	rVB	324669	420421	2.68%	0.254%
60	16.069	2185	2190	2198	rVB2	58608	95265	0.61%	0.058%
61	16.157	2200	2205	2209	rVB7	19805	28214	0.18%	0.017%
62	16.216	2212	2215	2221	rVV8	16870	28823	0.18%	0.017%
63	16.292	2226	2228	2237	rVB9	16381	32598	0.21%	0.020%
64	16.516	2263	2266	2270	rVB5	22952	29079	0.19%	0.018%
65	16.733	2299	2303	2307	rBV4	33060	48231	0.31%	0.029%
66	16.775	2307	2310	2316	rVV8	19010	39249	0.25%	0.024%
67	17.128	2367	2370	2375	rVB6	39264	47422	0.30%	0.029%
68	17.227	2384	2387	2391	rBV4	46118	64421	0.41%	0.039%
69	17.298	2396	2399	2402	rBV4	19881	20691	0.13%	0.012%
70	17.351	2402	2408	2417	rBV	3726879	5502711	35.02%	3.321%
71	17.451	2418	2425	2433	rBV	6618085	9682804	61.62%	5.844%
72	17.704	2465	2468	2472	rBV5	28439	38831	0.25%	0.023%
73	18.010	2516	2520	2524	rBV7	47927	67922	0.43%	0.041%
74	18.104	2532	2536	2540	rBV3	85263	129036	0.82%	0.078%
75	18.163	2542	2546	2550	rBV	213400	265065	1.69%	0.160%
76	18.222	2551	2556	2565	rBV	1090862	1469269	9.35%	0.887%

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77	18.798	2651	2654	2659	rBV2	61120	92955	0.59%	0.056%
78	19.257	2729	2732	2737	rVB2	85775	111665	0.71%	0.067%
79	19.333	2738	2745	2747	rBV2	212350	413060	2.63%	0.249%
80	19.445	2761	2764	2775	rVB3	194710	313679	2.00%	0.189%
81	19.680	2798	2804	2816	rBV	8646370	10949128	69.68%	6.609%
82	20.198	2888	2892	2904	rVB2	374591	679301	4.32%	0.410%
83	21.127	3045	3050	3052	rBV2	1633038	2472305	15.73%	1.492%
84	21.168	3053	3057	3064	rVB4	1534882	3800871	24.19%	2.294%
85	21.433	3097	3102	3106	rBV	4644028	6690401	42.58%	4.038%
86	21.498	3110	3113	3114	rBV	644120	696153	4.43%	0.420%
87	23.127	3387	3390	3397	rVB	550859	807146	5.14%	0.487%
88	23.757	3489	3497	3511	rVB2	6352735	13208107	84.05%	7.972%
89	23.915	3517	3524	3532	rVB2	3171223	6407213	40.77%	3.867%
90	24.427	3603	3611	3622	rVB	7257436	15714070	100.00%	9.485%
91	24.715	3655	3660	3671	rVB4	837781	1903435	12.11%	1.149%

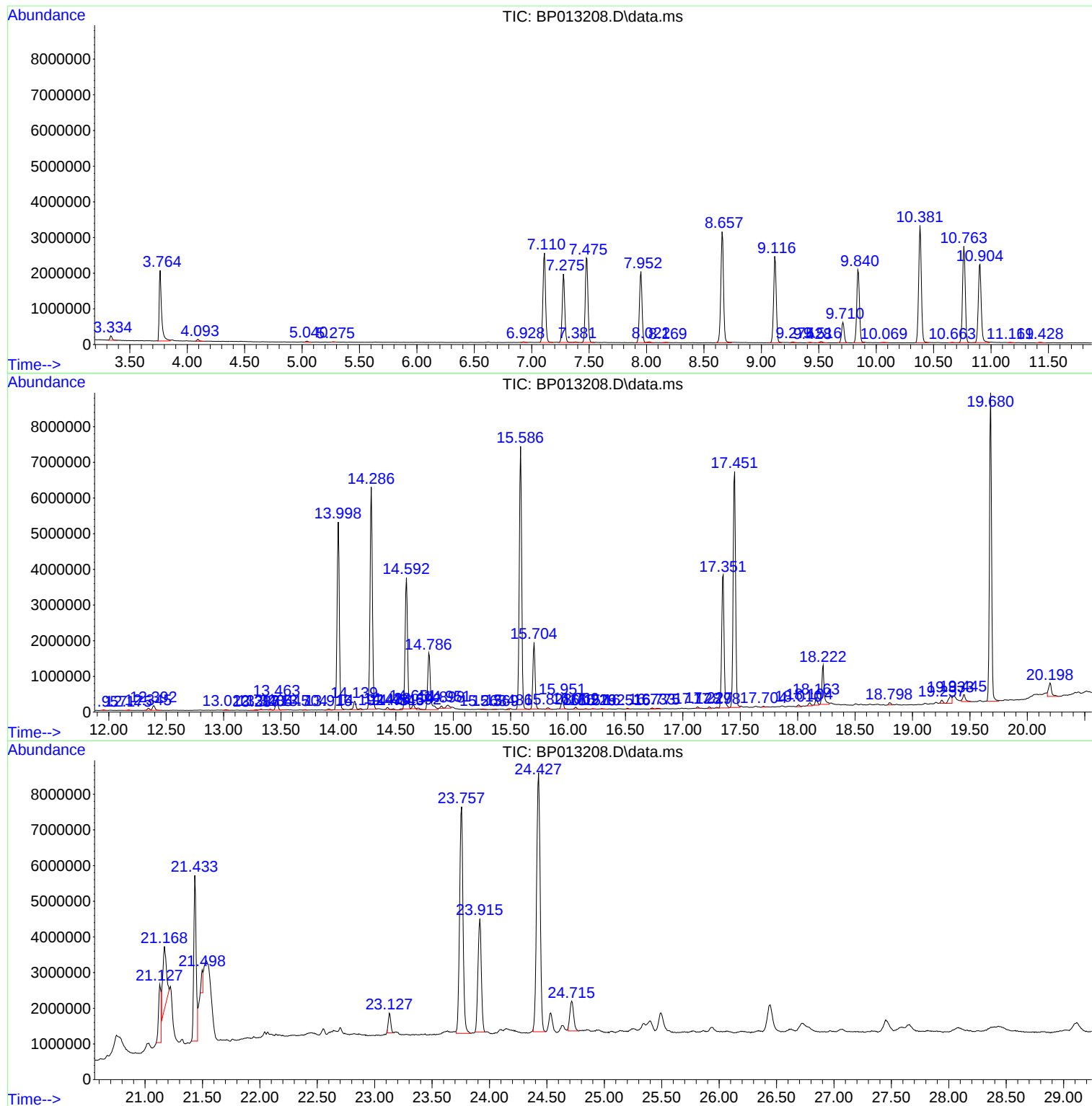
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



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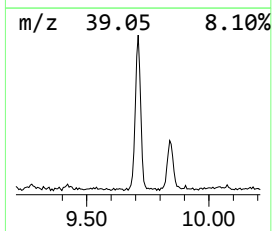
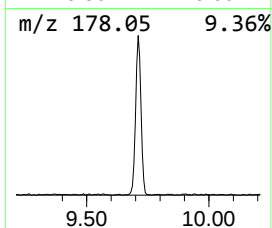
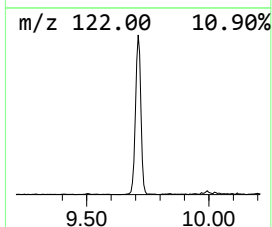
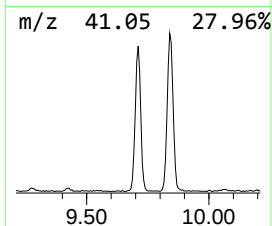
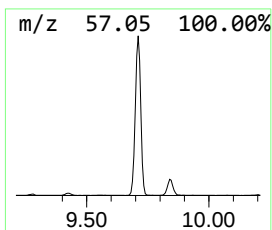
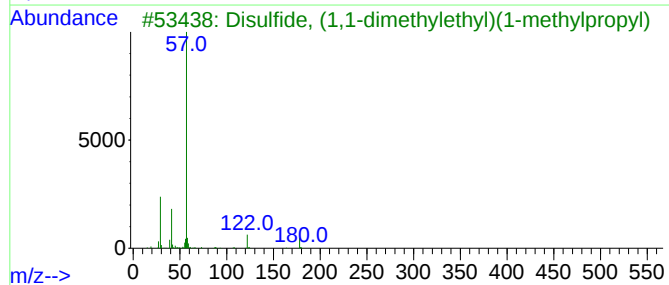
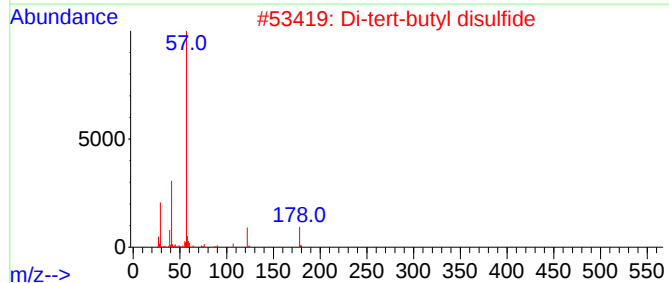
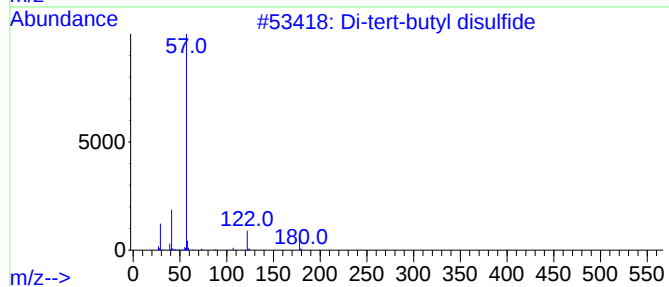
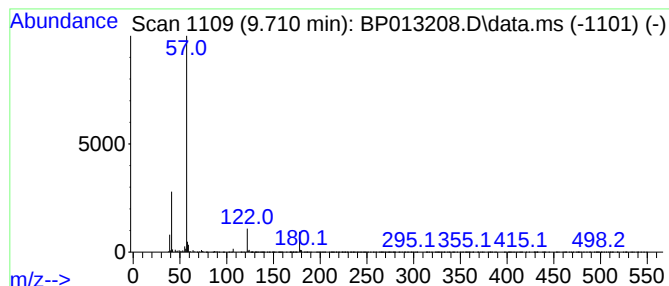
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Di-tert-butyl disulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	4.03 ng/ul	894631	Naphthalene-d8	10.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	91
2			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	87
3			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	80
4			Disulfide, dibutyl	178	C8H18S2	000629-45-8	72
5			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	52



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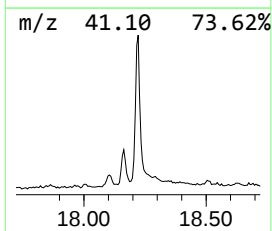
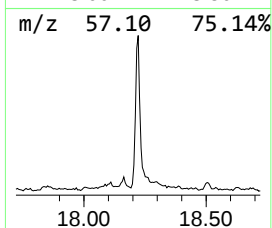
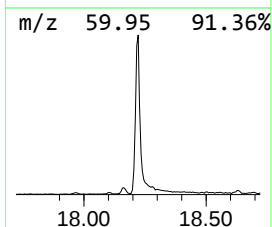
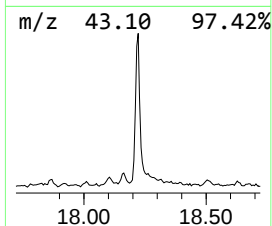
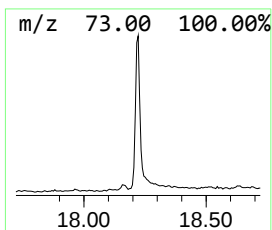
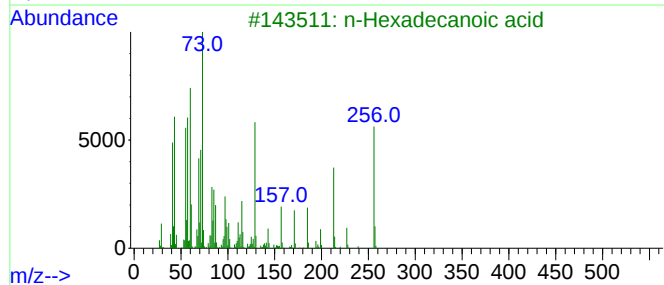
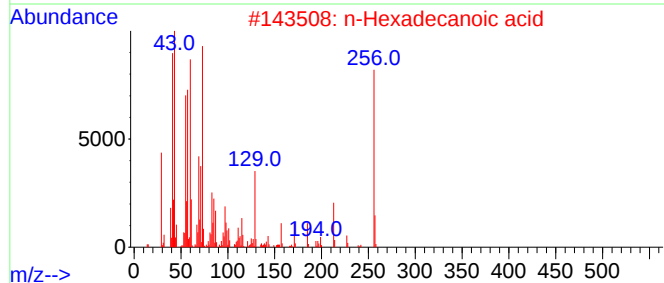
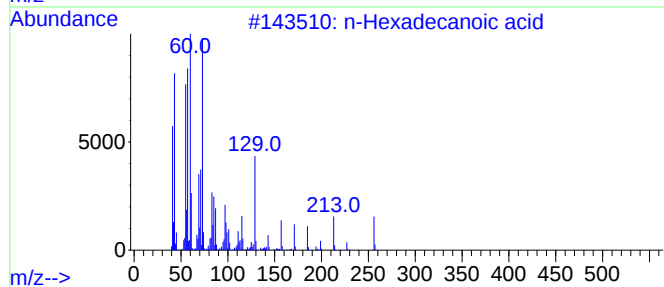
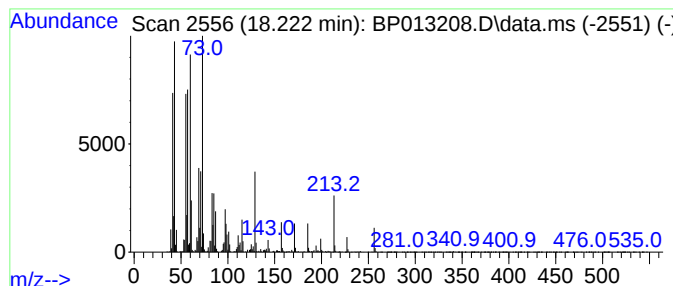
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	5.34 ng/ul	1469270	Phenanthrene-d10	17.351

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	92
4			Octadecanoic acid	284	C18H36O2	000057-11-4	90
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	90



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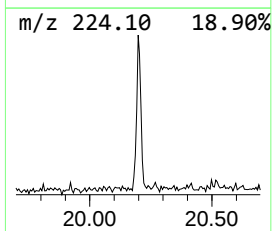
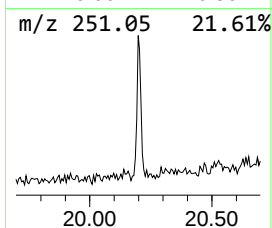
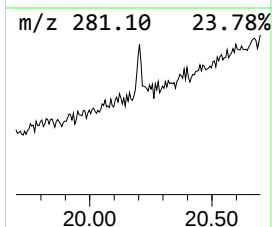
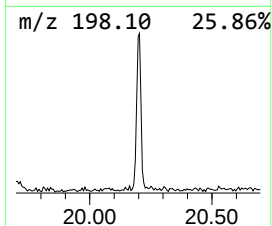
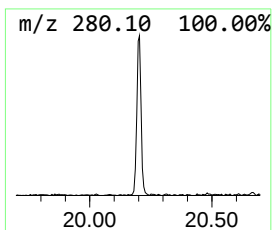
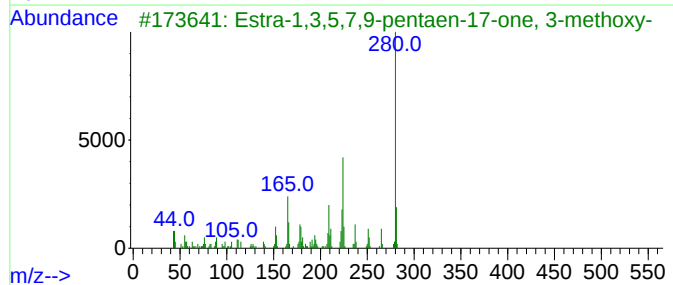
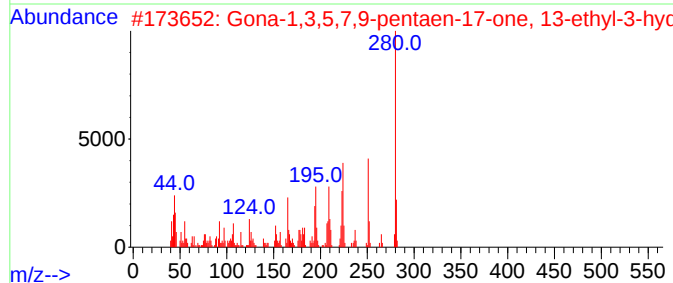
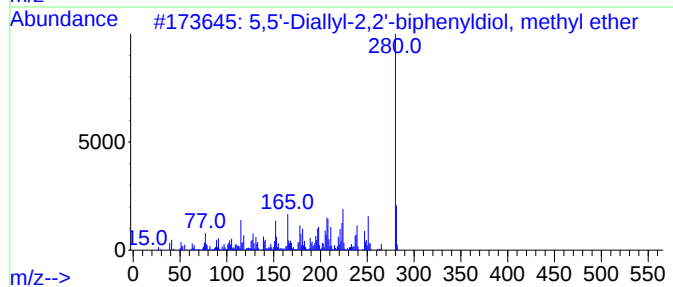
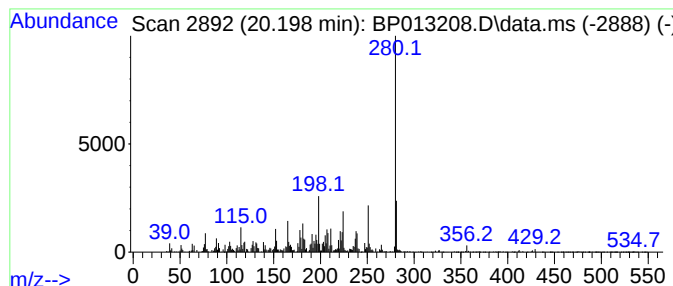
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 5,5'-Diallyl-2,2'-biphenyld... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.198	2.03 ng/ul	679301	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,5'-Diallyl-2,2'-biphenyldiol, ...	280	C19H20O2	1000384-18-6	74
2			Gona-1,3,5,7,9-pentaen-17-one, 1...	280	C19H20O2	030788-51-3	64
3			Estra-1,3,5,7,9-pentaen-17-one, ...	280	C19H20O2	003907-67-3	64
4			Silane, dimethyl(2-propylphenoxy...	280	C16H28O2Si	1000347-41-5	62
5			N-Butyl-4-hydrazino-6-(2,2,2-tri...	280	C9H15F3N6O	1000389-26-8	50



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Instrument :
BNA_P
ClientSampleId :
DBXR5

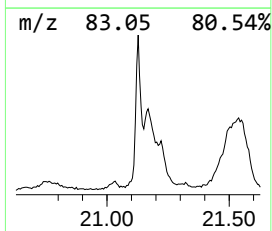
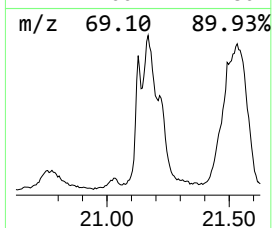
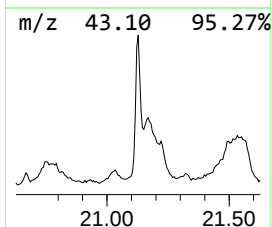
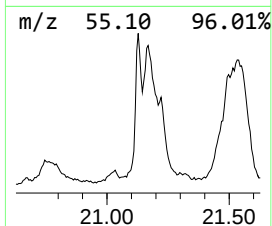
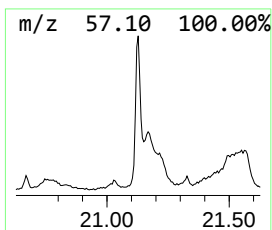
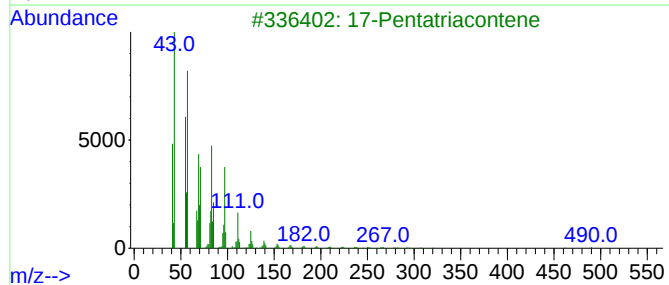
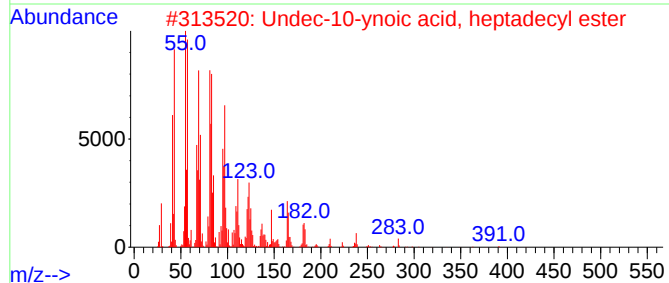
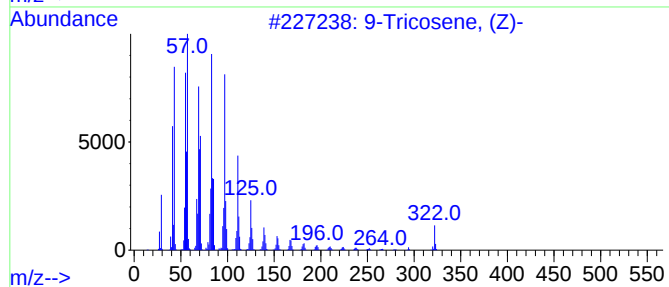
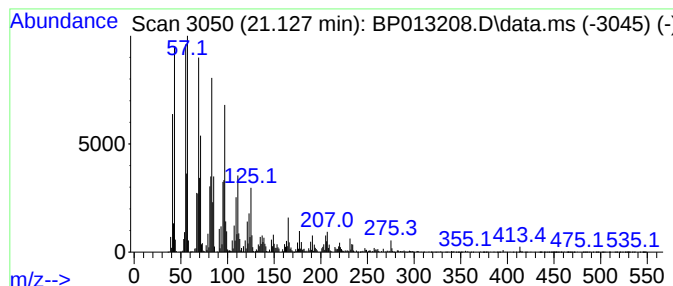
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	7.39 ng/ul	2472310	Chrysene-d12	21.433

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
2		Undec-10-ynoic acid, heptadecyl ...	420	C28H52O2	1000406-17-0	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	87
4		1-Hexacosanol	382	C26H54O	000506-52-5	83
5		1-Hexacosanol	382	C26H54O	000506-52-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013208.D
Acq On : 21 Dec 2022 15:12
Operator : CG/JU
Sample : N6014-04
Misc :
ALS Vial : 90 Sample Multiplier: 1

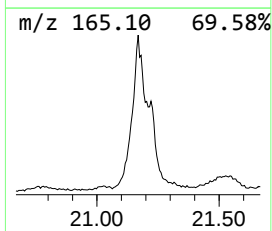
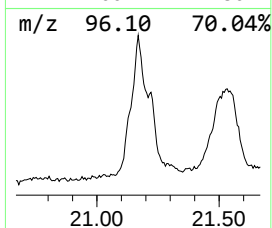
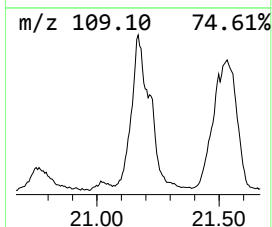
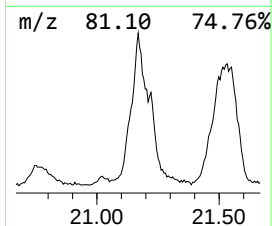
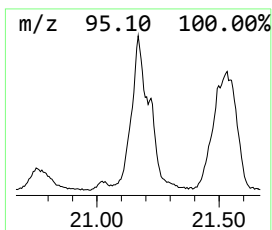
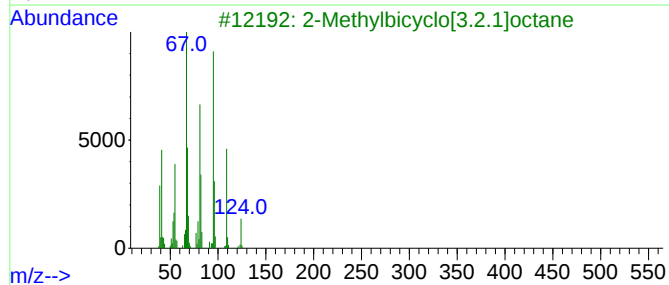
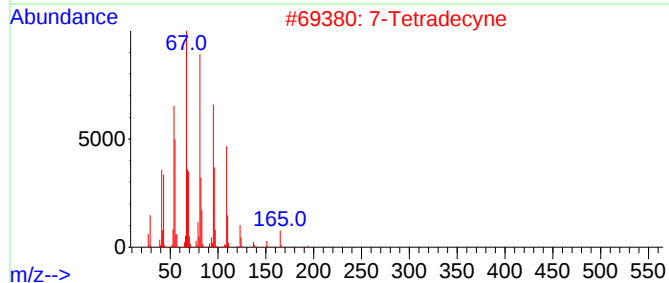
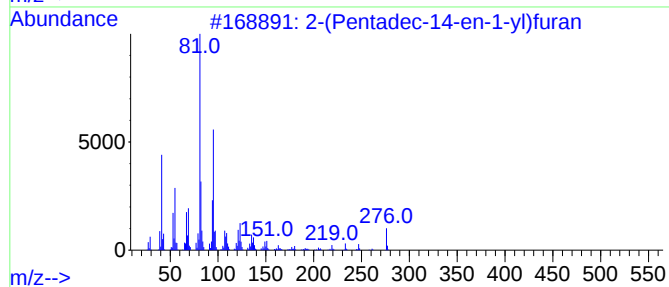
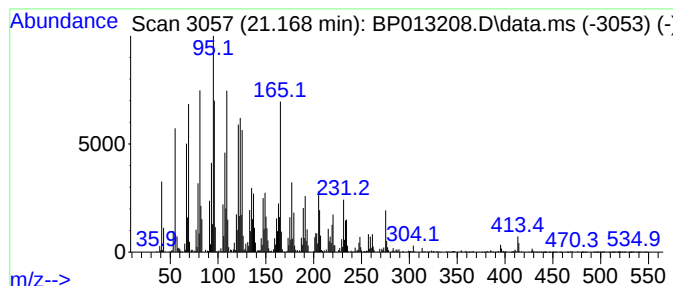
Instrument :
BNA_P
ClientSampleId :
DBXR5

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 5 2-(Pentadec-14-en-1-yl)furan Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.169	11.36 ng/ul	3800870	Chrysene-d12	21.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Pentadec-14-en-1-yl)furan	276	C19H32O	1000465-69-5	64
2	7-Tetradecyne	194	C14H26	035216-11-6	52
3	2-Methylbicyclo[3.2.1]octane	124	C9H16	1010215-28-0	46
4	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	45
5	3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013208.D
Acq On : 21 Dec 2022 15:12
Operator : CG/JU
Sample : N6014-04
Misc :
ALS Vial : 90 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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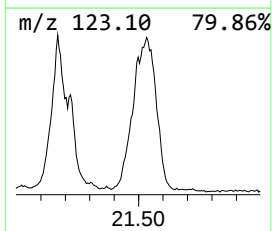
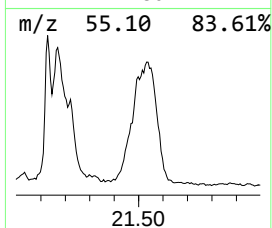
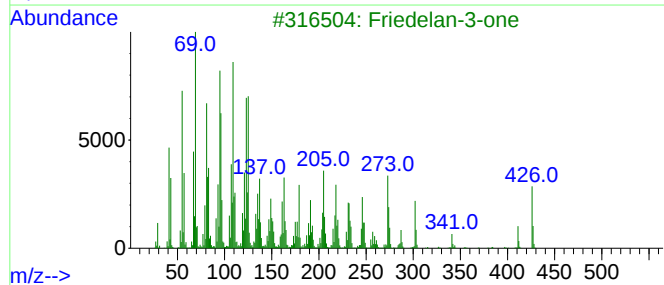
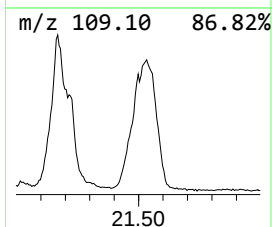
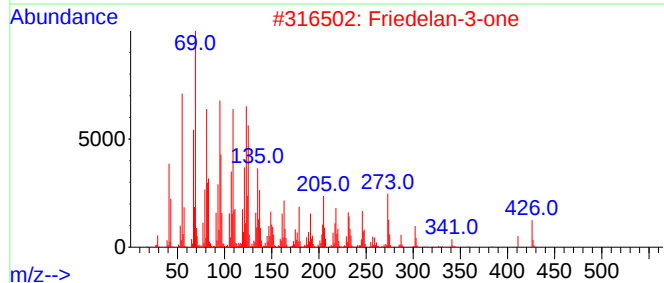
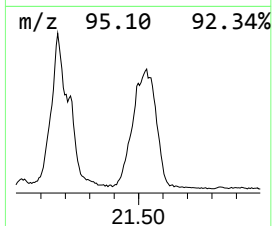
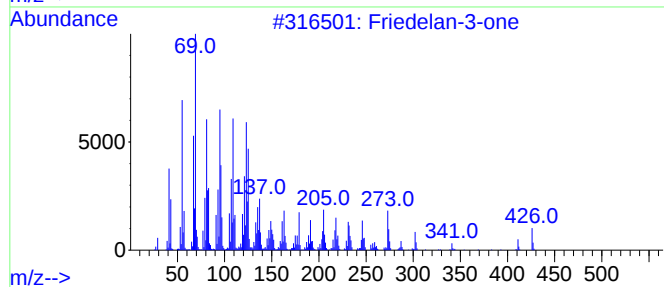
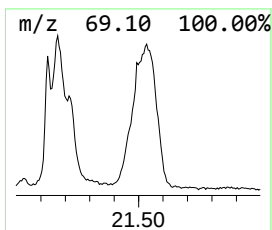
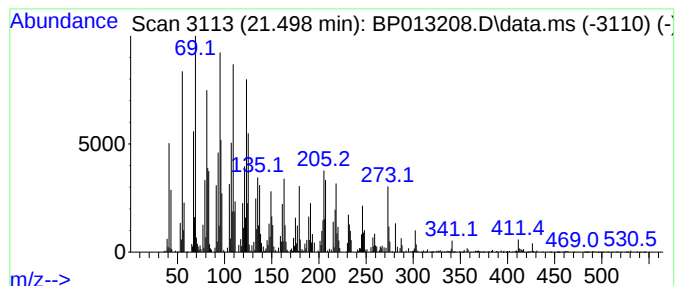
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 D:A-Friedooleanan-3-ol, (3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.498	2.08 ng/ul	696153	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	89
2			Friedelan-3-one	426	C30H50O	000559-74-0	64
3			Friedelan-3-one	426	C30H50O	000559-74-0	62
4			D:A-Friedooleanan-3-ol, (3.alpha.)-	428	C30H52O	005085-72-3	58
5			Azulene, 1,2,3,3a,4,5,6,7-octahy...	204	C15H24	022567-17-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013208.D
Acq On : 21 Dec 2022 15:12
Operator : CG/JU
Sample : N6014-04
Misc :
ALS Vial : 90 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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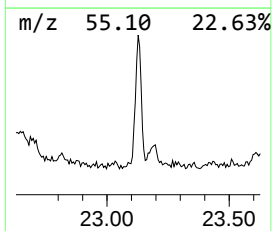
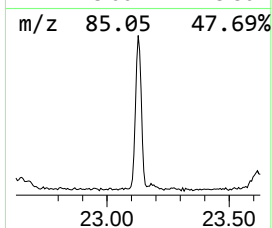
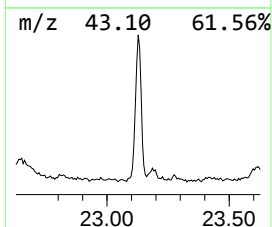
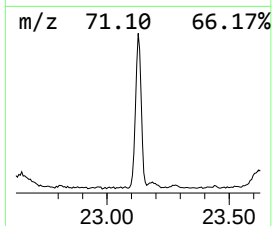
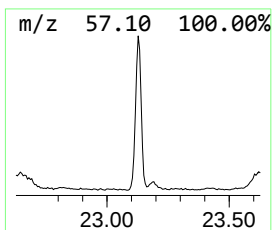
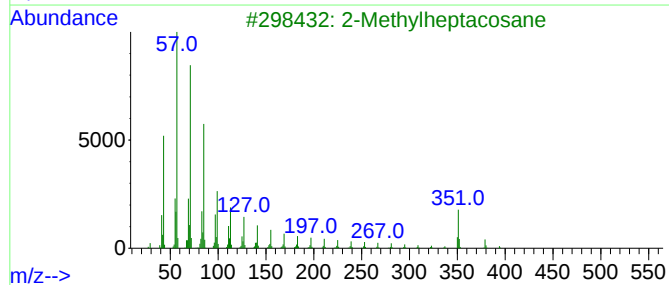
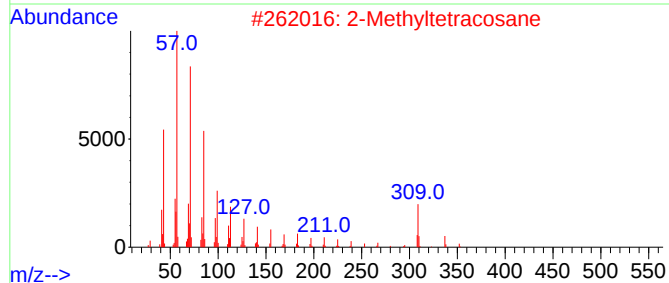
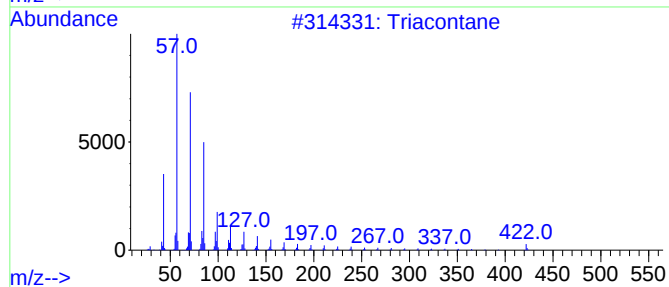
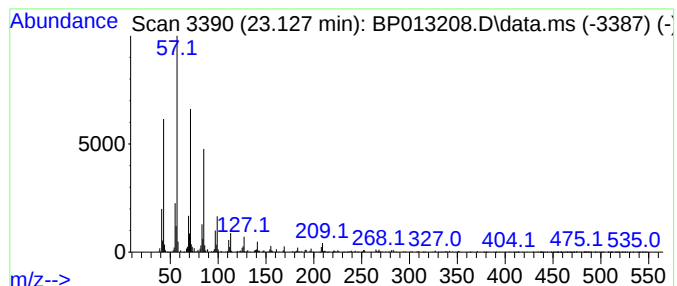
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.127	2.52 ng/ul	807146	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triaccontane	422	C30H62	000638-68-6	97
2			2-Methyltetracosane	352	C25H52	001560-78-7	93
3			2-Methylheptacosane	394	C28H58	001561-00-8	93
4			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	87
5			Triaccontane, 1-iodo-	548	C30H61I	1000406-32-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013208.D
Acq On : 21 Dec 2022 15:12
Operator : CG/JU
Sample : N6014-04
Misc :
ALS Vial : 90 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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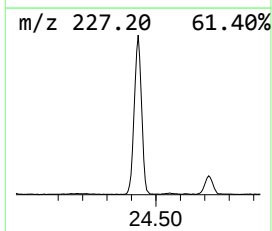
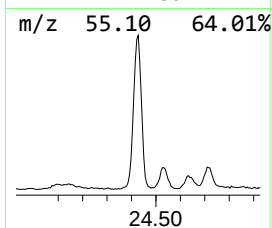
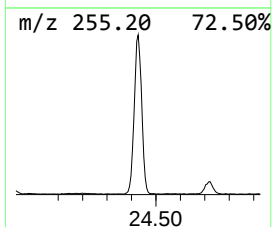
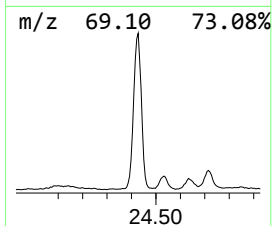
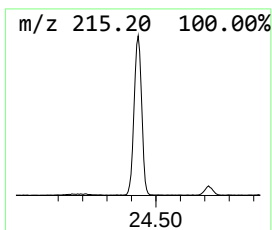
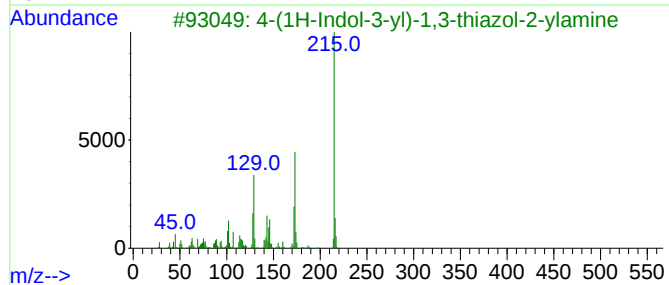
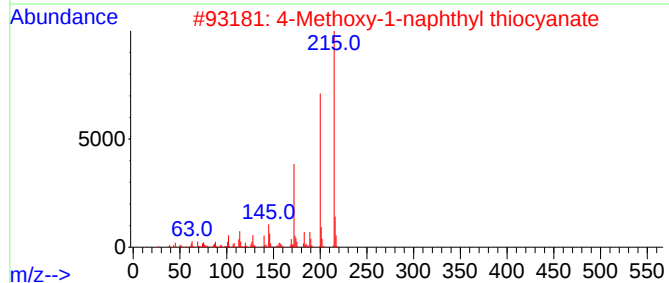
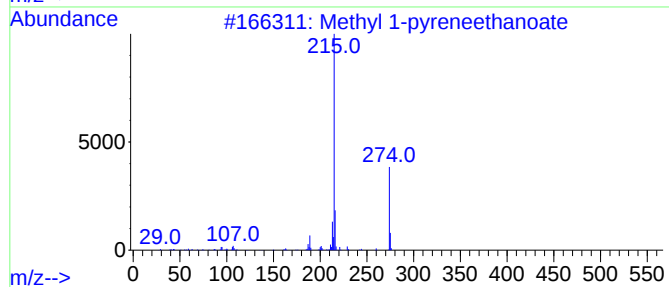
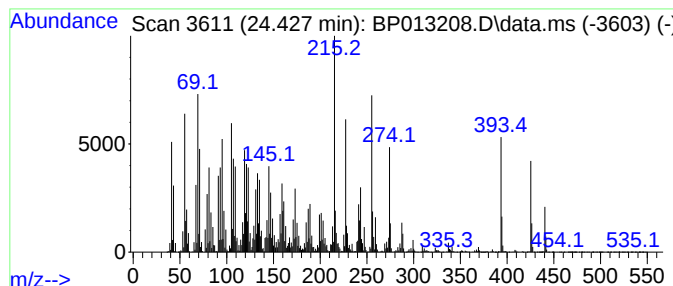
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Methyl 1-pyreneethanoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.427	49.05 ng/ul	15714100	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	52
2			4-Methoxy-1-naphthyl thiocyanate	215	C12H9NOS	066231-77-4	18
3			4-(1H-Indol-3-yl)-1,3-thiazol-2-...	215	C11H9N3S	022258-56-6	18
4			1-Pyrenebutanoic acid	288	C20H16O2	003443-45-6	15
5			N-[2-(1H-Indol-3-yl)ethyl]propan...	288	C16H24N2OSi	1000493-19-0	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013208.D
Acq On : 21 Dec 2022 15:12
Operator : CG/JU
Sample : N6014-04
Misc :
ALS Vial : 90 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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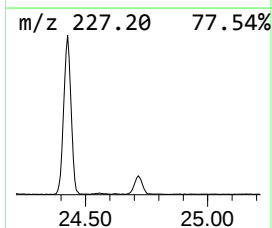
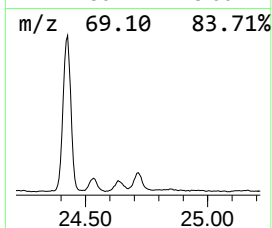
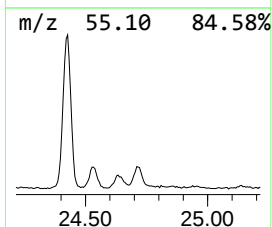
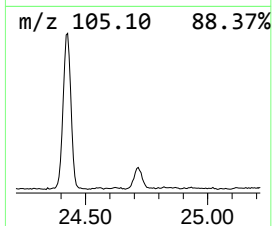
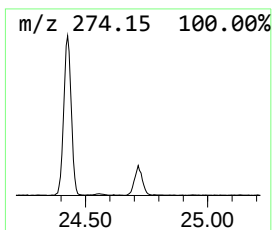
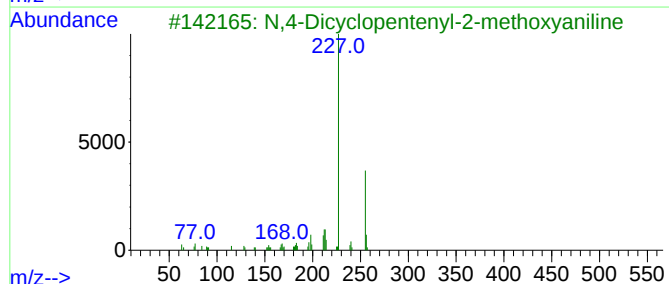
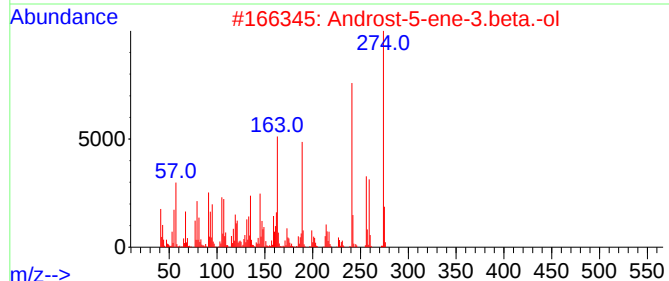
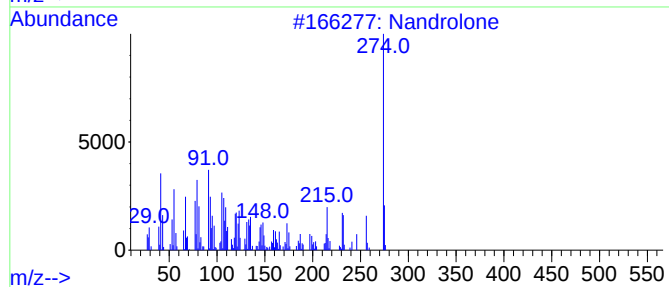
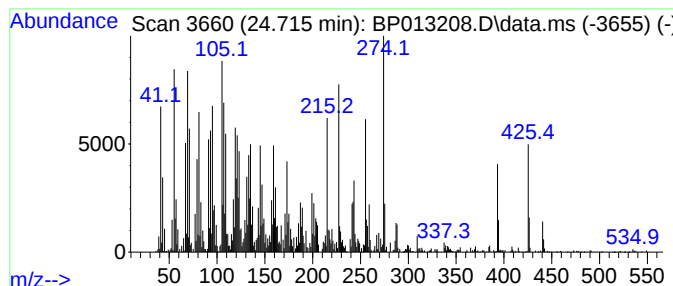
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.715	5.94 ng/ul	1903440	Perylene-d12	23.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nandrolone	274	C18H26O2	000434-22-0	47
2			Androst-5-ene-3.beta.-ol	274	C19H30O	001476-64-8	46
3			N,4-Dicyclopentenyl-2-methoxyani...	255	C17H21NO	1000441-76-4	35
4			Silane, dimethyl(2-naphthoxy)but...	274	C16H22O2Si	1000347-21-1	25
5			Dicyclopenta[a,d]benzene, 4,8-di...	242	C18H26	1000156-41-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013208.D
Acq On : 21 Dec 2022 15:12
Operator : CG/JU
Sample : N6014-04
Misc :
ALS Vial : 90 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR5

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
Di-tert-butyl d...	9.710	4.0	ng/ul	894631	2	10.763	4443750	20.0
n-Hexadecanoic ...	18.222	5.3	ng/ul	1469270	4	17.351	5502710	20.0
5,5'-Diallyl-2,...	20.198	2.0	ng/ul	679301	5	21.433	6690400	20.0
(DEL) Alkane: S...	21.127	7.4	ng/ul	2472310	5	21.433	6690400	20.0
2-(Pentadec-14-...	21.169	11.4	ng/ul	3800870	5	21.433	6690400	20.0
D:A-Friedoolean...	21.498	2.1	ng/ul	696153	5	21.433	6690400	20.0
(DEL) Alkane: S...	23.127	2.5	ng/ul	807146	6	23.915	6407210	20.0
Methyl 1-pyrene...	24.427	49.0	ng/ul	15714100	6	23.915	6407210	20.0
unknown-01	24.715	5.9	ng/ul	1903440	6	23.915	6407210	20.0