LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032023\
Data File : BP014155.D
Acq On : 20 Mar 2023 23:36
Operator : CG/JU
Sample : 01885-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB907

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-BP030723.M
Title : SVOA CALIBRATION

Signal : TIC: BP014155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.417	35	39	42	rBV	39475	54836	0.80%	0.077%
2	3.452	42	45	51	rVB	42703	56502	0.82%	0.080%
3	3.852	110	113	136	rBV	243064	430386	6.25%	0.607%
4	4.075	148	151	157	rVB4	6976	9789	0.14%	0.014%
5	4.175	164	168	175	rVB	15448	23775	0.35%	0.034%
6	4.481	217	220	225	rBV7	3533	7375	0.11%	0.010%
7	4.634	238	246	256	rBV	82589	132580	1.93%	0.187%
8	5.334	361	365	369	rVB	7204	9237	0.13%	0.013%
9	5.593	406	409	418	rVB	5839	13674	0.20%	0.019%
10	5.728	427	432	436	rBV7	4005	8921	0.13%	0.013%
11	5.969	467	473	478	rVB9	3787	7435	0.11%	0.010%
12	6.928	629	636	643	rBV9	5174	10627	0.15%	0.015%
13	7.211	676	684	695	rBV	211403	375367	5.45%	0.529%
14	7.375	705	712	726	rBV	798339	1281015	18.62%	1.806%
15	7.581	740	747	755	rBV	769762	1256297	18.26%	1.771%
16	7.640	755	757	763	rVV5	13295	21534	0.31%	0.030%
17	7.699	763	767	776	rVB5	5666	14422	0.21%	0.020%
18	7.911	794	803	806	rBV8	8953	18199	0.26%	0.026%
19	8.052	819	827	835	rBV	810299	1298437	18.87%	1.830%
20	8.146	841	843	848	rVB5	6200	7732	0.11%	0.011%
21	8.358	875	879	883	rBV5	6250	9298	0.14%	0.013%
22	8.428	886	891	903	rVV2	29867	60681	0.88%	0.086%
23	8.534	903	909	914	rVB10	5346	11523	0.17%	0.016%
24	8.763	934	948	958	rBV	662795	1130670	16.43%	1.594%
25	8.893	968	970	976	rVB7	5030	7223	0.10%	0.010%
26	8.969	979	983	990	rVB10	4828	10874	0.16%	0.015%
27	9.163	1011	1016	1019	rBV6	6733	9345	0.14%	0.013%
28	9.222	1019	1026	1040	rBV	1031819	1756540	25.53%	2.476%
29	9.363	1048	1050	1056	rVB6	4125	7021	0.10%	0.010%
30	9.440	1056	1063	1068	rVV9	8648	19101	0.28%	0.027%
31	9.510	1071	1075	1079	rVV2	8433	13256	0.19%	0.019%
32	9.581	1079	1087	1098	rVV2	84165	169858	2.47%	0.239%
33	9.675	1098	1103	1110	rVB4	30042	65823	0.96%	0.093%
34	9.805	1120	1125	1130	rVB5	15229	22188	0.32%	0.031%
35	9.863	1131	1135	1143	rVB5	7699	17129	0.25%	0.024%
36	9.952	1143	1150	1161	rBV	854721	1454756	21.14%	2.050%

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Misc :
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Instrument :
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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

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Title : SVOA CALIBRATION

37	10.052	1163	1167	1170	rBV5	6985	10752	0.16%	0.015%
38	10.152	1181	1184	1191	rVB9	8405	14643	0.21%	0.021%
39	10.216	1191	1195	1198	rBV6	6401	10952	0.16%	0.015%
40	10.263	1199	1203	1209	rVB8	10069	19981	0.29%	0.028%
41	10.399	1220	1226	1229	rBV7	8332	15286	0.22%	0.022%
42	10.493	1235	1242	1263	rBV	1193159	2113149	30.71%	2.978%
43	10.657	1263	1270	1274	rVV10	8792	21330	0.31%	0.030%
44	10.705	1274	1278	1282	rVV6	8320	14611	0.21%	0.021%
45	10.775	1286	1290	1294	rVV6	5843	7924	0.12%	0.011%
46	10.875	1300	1307	1319	rVB	1124952	1901017	27.63%	2.679%
47	11.010	1323	1330	1349	rBV	519783	1050322	15.26%	1.480%
48	11.428	1394	1401	1403	rBV6	9959	19006	0.28%	0.027%
49	11.463	1405	1407	1414	rVB8	9498	14056	0.20%	0.020%
50	11.581	1422	1427	1435	rVB2	38663	68244	0.99%	0.096%
51	11.675	1439	1443	1445	rBV5	8846	12839	0.19%	0.018%
52	11.846	1468	1472	1475	rBV5	7150	9961	0.14%	0.014%
53	11.922	1481	1485	1492	rVB10	9590	21194	0.31%	0.030%
54	12.069	1503	1510	1516	rBV9	15877	38589	0.56%	0.054%
55	12.122	1516	1519	1524	rVB5	21398	34784	0.51%	0.049%
56	12.204	1524	1533	1538	rBV	126462	235606	3.42%	0.332%
57	12.252	1538	1541	1547	rVB6	16736	29511	0.43%	0.042%
58	12.463	1569	1577	1588	rBV5	26083	93188	1.35%	0.131%
59	12.628	1601	1605	1610	rBV4	20061	32776	0.48%	0.046%
60	12.951	1655	1660	1664	rBV7	10623	23691	0.34%	0.033%
61	13.387	1731	1734	1737	rBV4	12791	19801	0.29%	0.028%
62	13.499	1749	1753	1755	rBV5	16104	24241	0.35%	0.034%
63	13.651	1775	1779	1783	rVB6	14242	20654	0.30%	0.029%
64	13.869	1812	1816	1819	rBV5	19960	28038	0.41%	0.040%
65	13.910	1819	1823	1826	rVV5	34478	53010	0.77%	0.075%
66	13.951	1827	1830	1835	rVB	32689	49879	0.72%	0.070%
67	14.010	1837	1840	1842	rBV4	12165	16741	0.24%	0.024%
68	14.098	1848	1855	1862	rVB	2493733	3556486	51.68%	5.013%
69	14.246	1877	1880	1883	rBV5	15479	22681	0.33%	0.032%
70	14.304	1887	1890	1897	rVV9	33200	67777	0.98%	0.096%
71	14.387	1898	1904	1915	rVB	2841230	4152292	60.34%	5.853%
72	14.493	1917	1922	1931	rVV	150439	262185	3.81%	0.370%
73	14.610	1938	1942	1945	rBV5	50336	74991	1.09%	0.106%
74	14.693	1950	1956	1962	rVV	1823012	2634097	38.28%	3.713%
75	14.904	1988	1992	2003	rBV	150939	302641	4.40%	0.427%
76	15.057	2014	2018	2022	rBV4	60395	115285	1.68%	0.162%

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77	15.434	2077	2082	2087	rBV2	47481	103364	1.50%	0.146%
78	15.687	2118	2125	2137	rVB	3603832	5300699	77.03%	7.471%
79	15.804	2139	2145	2152	rBV	1348578	1891133	27.48%	2.666%
80	15.892	2156	2160	2164	rBV	201289	247047	3.59%	0.348%
81	16.045	2181	2186	2194	rBV	188412	260414	3.78%	0.367%
82	16.204	2206	2213	2222	rBV	2500108	3520208	51.16%	4.962%
83	16.528	2264	2268	2274	rVB	130769	172717	2.51%	0.243%
84	16.716	2294	2300	2305	rBV	1522929	2103418	30.57%	2.965%
85	16.828	2316	2319	2324	rBV7	33037	68414	0.99%	0.096%
86	17.445	2418	2424	2431	rBV	2289460	3278384	47.64%	4.621%
87	17.545	2435	2441	2448	rBV	3965502	5523914	80.27%	7.786%
88	18.304	2566	2570	2580	rBV	738422	1020473	14.83%	1.438%
89	19.528	2775	2778	2789	rVB	298891	410304	5.96%	0.578%
90	19.769	2813	2819	2823	rBV	5116354	6881285	100.00%	9.699%
91	19.804	2823	2825	2834	rVB	290719	359108	5.22%	0.506%
92	20.733	2980	2983	2987	rBV2	151941	170010	2.47%	0.240%
93	21.198	3058	3062	3069	rBV	772054	942922	13.70%	1.329%
94	21.527	3112	3118	3125	rBV	2389151	3370537	48.98%	4.751%
95	22.792	3330	3333	3339	rVB	242419	344584	5.01%	0.486%
96	23.880	3511	3518	3527	rVB2	2448850	5091778	73.99%	7.177%
97	24.045	3540	3546	3555	rVB2	1406721	2869343	41.70%	4.044%

Sum of corrected areas: 70947693

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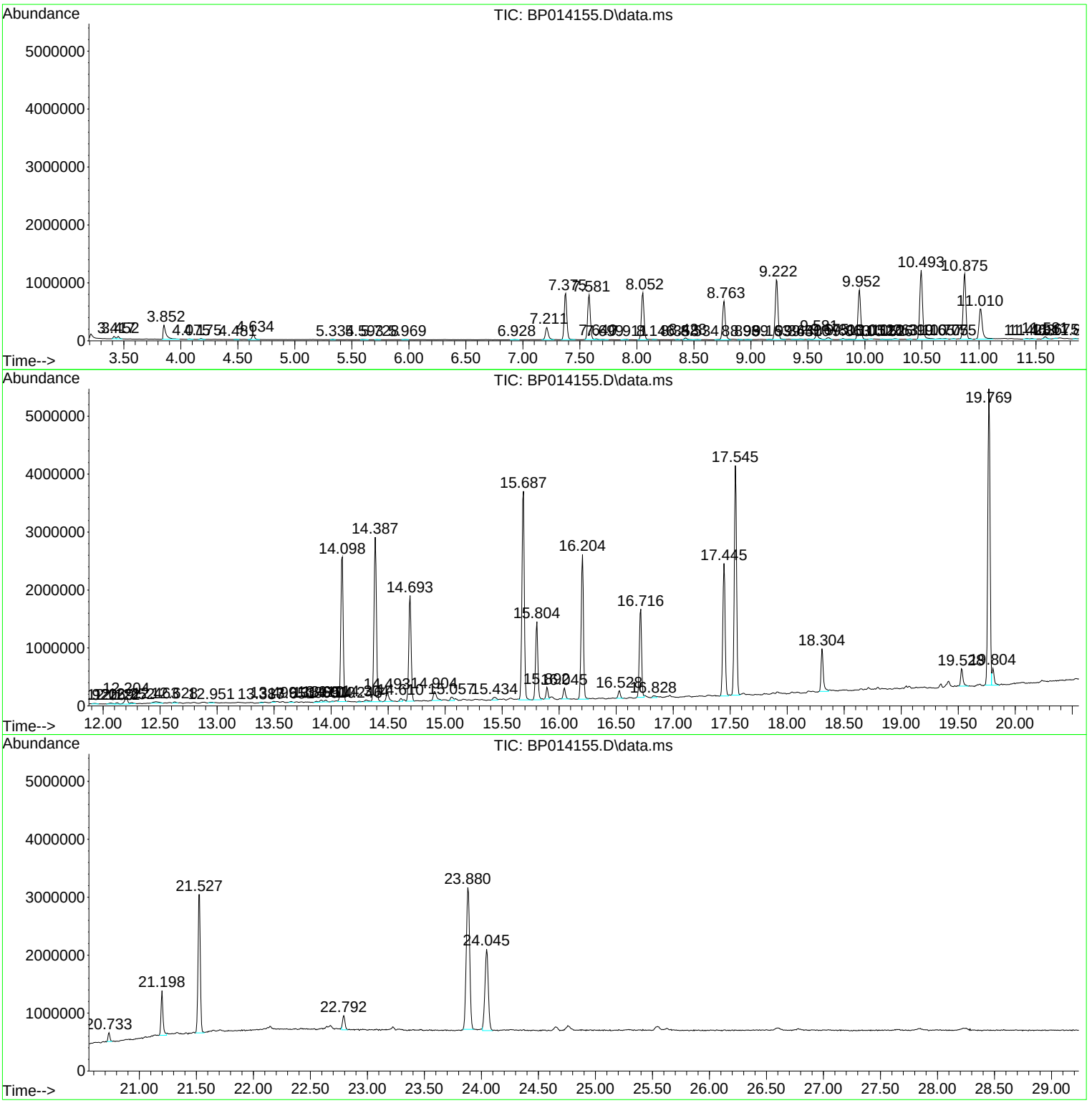
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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



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Quant Title : SVOA CALIBRATION

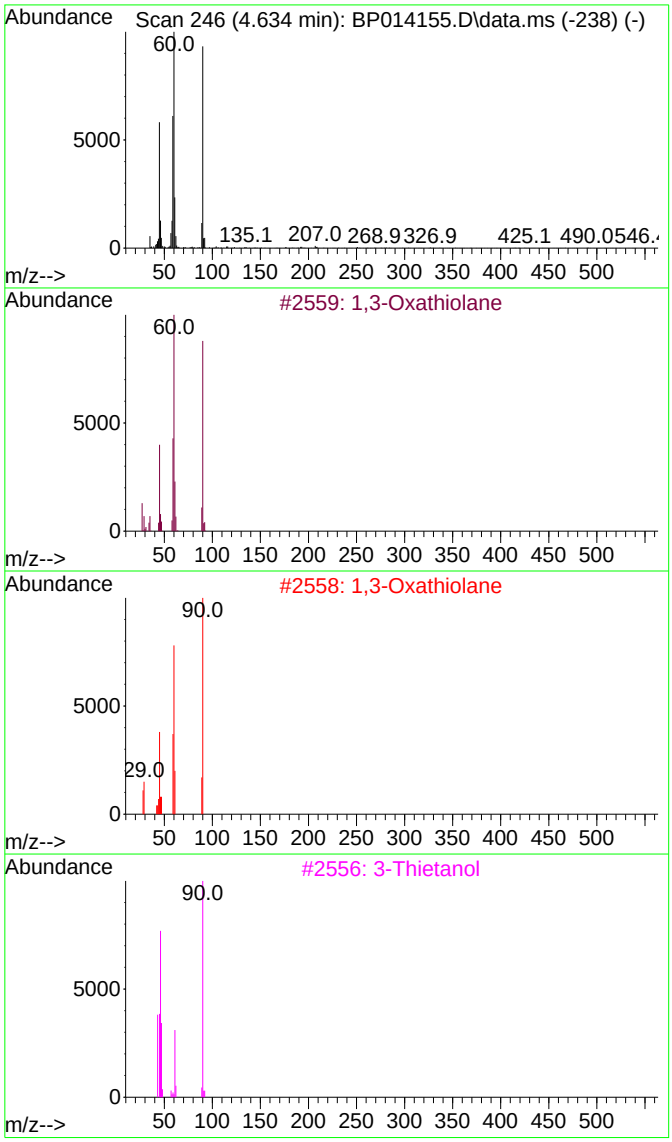
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

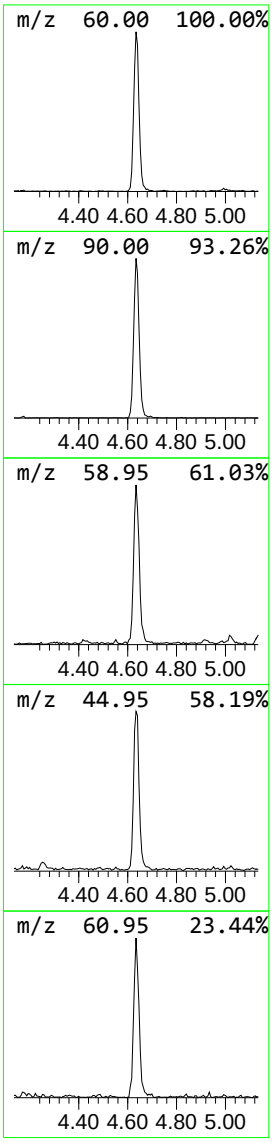
****

Peak Number 1 1,3-Oxathiolane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.634	2.04 ng/ul	132580	1,4-Dichlorobenzene-d4	8.052

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane	90	C3H6OS	002094-97-5	94
2	1,3-Oxathiolane	90	C3H6OS	002094-97-5	83
3	3-Thietanol	90	C3H6OS	010304-16-2	53
4	Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
5	2,3-Dimercaptopropan-1-ol	124	C3H8OS2	000059-52-9	39





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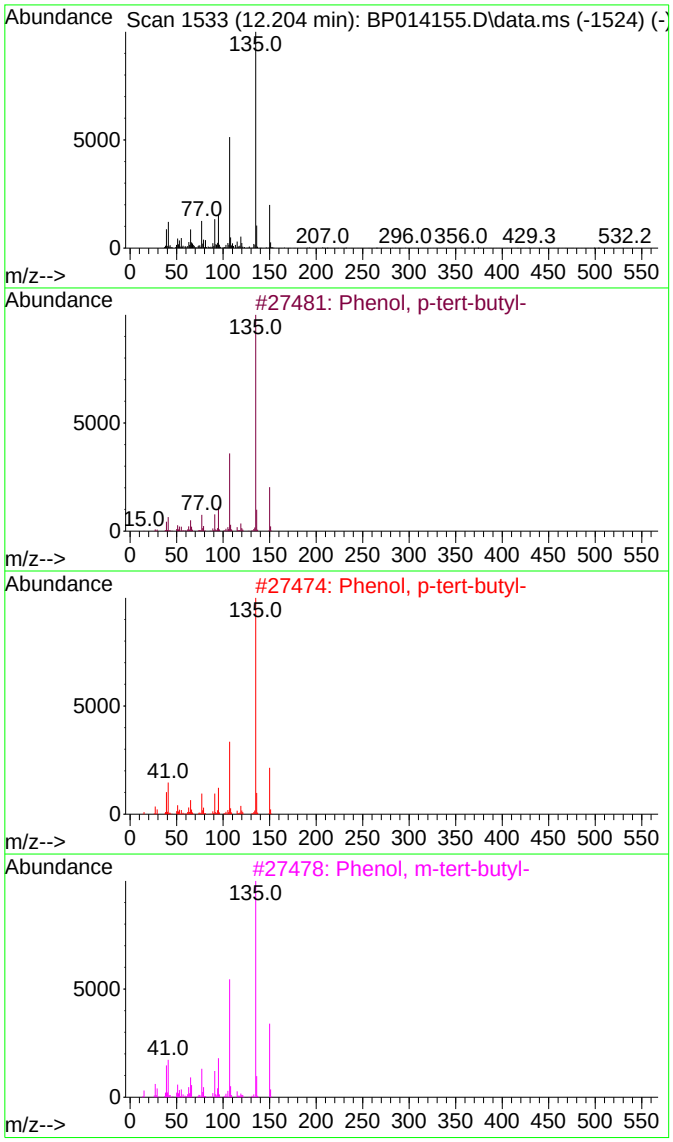
Quant Title : SVOA CALIBRATION

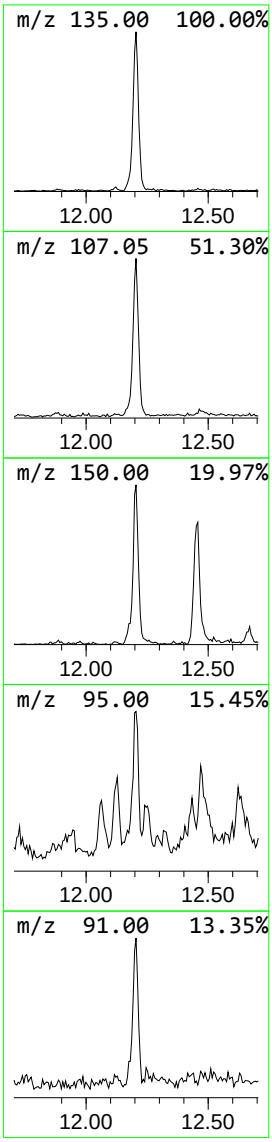
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Phenol, p-tert-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.204	2.48 ng/ul	235606	Naphthalene-d8	10.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	87





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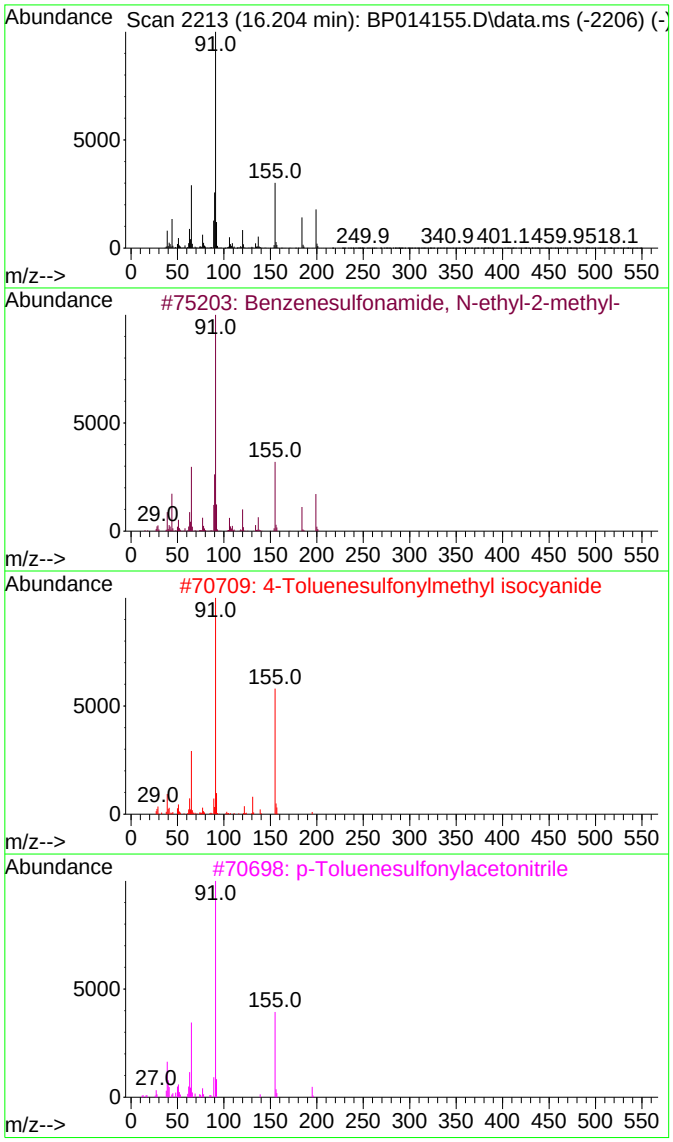
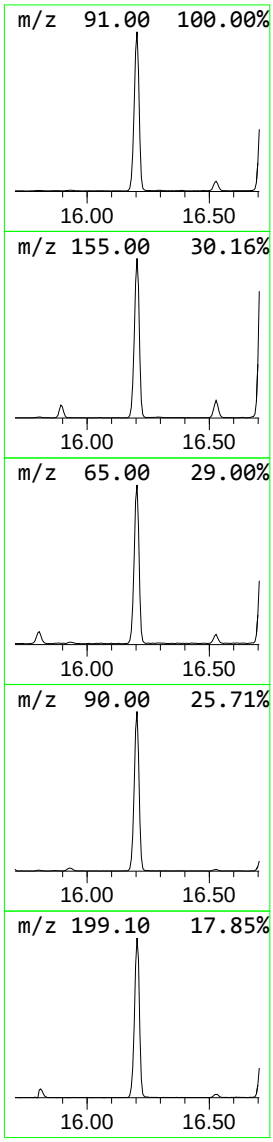
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzenesulfonamide, N-ethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	21.48 ng/ul	3520210	Phenanthrene-d10	17.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-2-me...	199	C9H13NO2S	001077-56-1	98
2	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	52
3	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	50
4	Tolbutamide	270	C12H18N2O3S	000064-77-7	50
5	1-Hydroxytricyclo[4.3.0.0(4,9)]n...	308	C16H20O4S	201992-83-8	50





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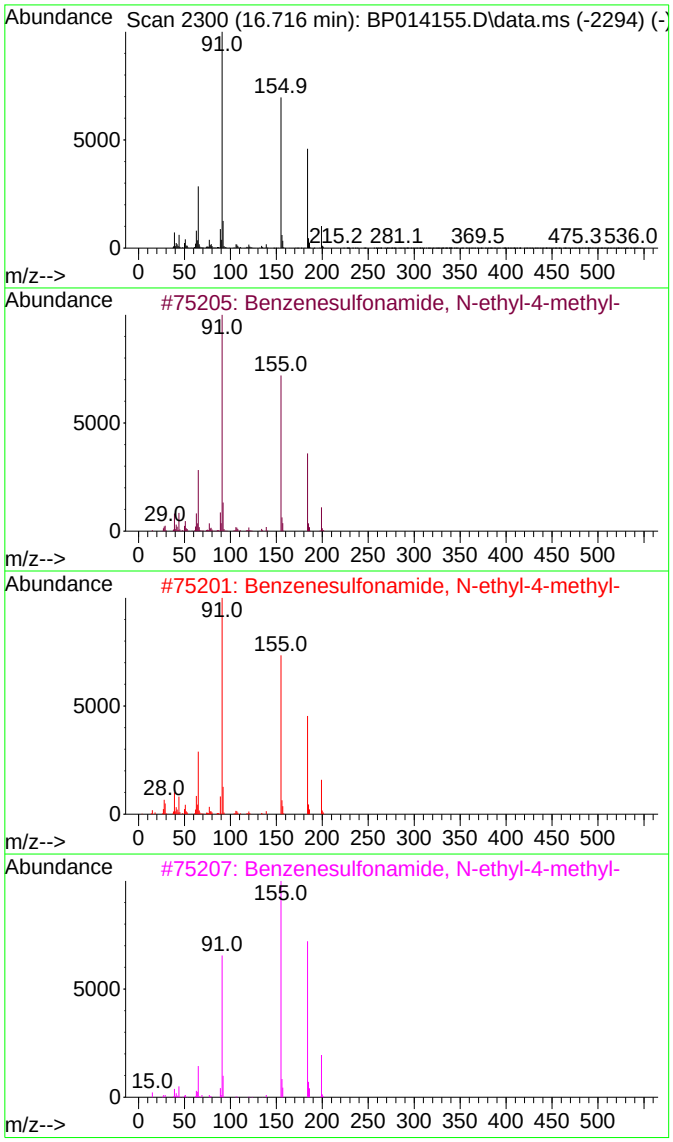
Quant Title : SVOA CALIBRATION

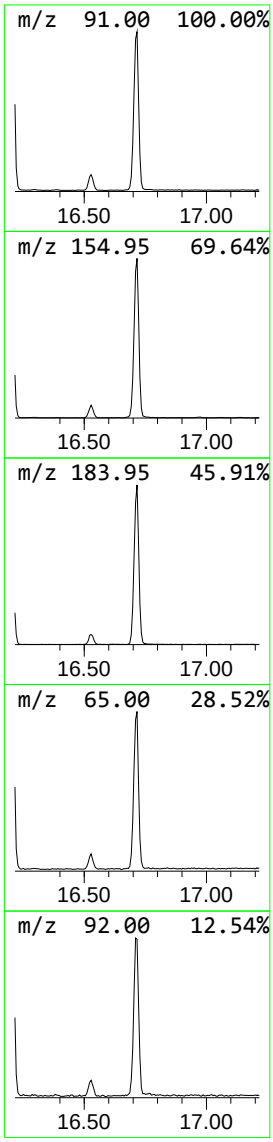
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzenesulfonamide, N-ethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.716	12.83 ng/ul	2103420	Phenanthrene-d10	17.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	97
2	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	95
3	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	91
4	N-isobutyl-4-methylbenzenesulfon...	227	C11H17NO2S	023705-38-6	86
5	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	81





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BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

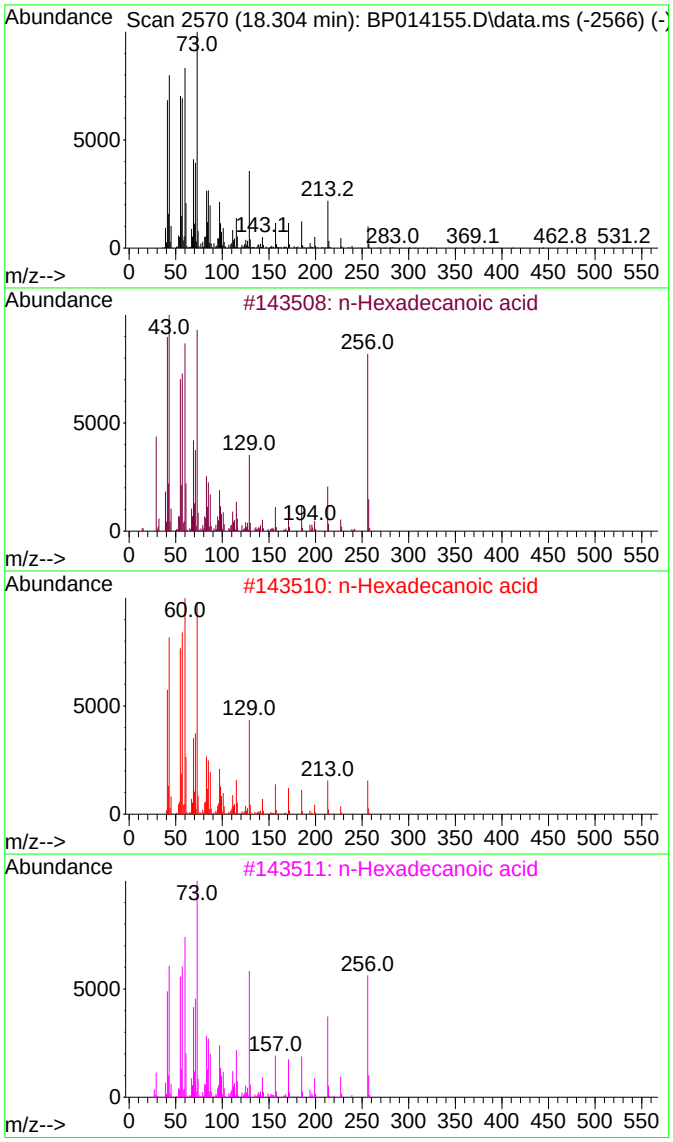
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

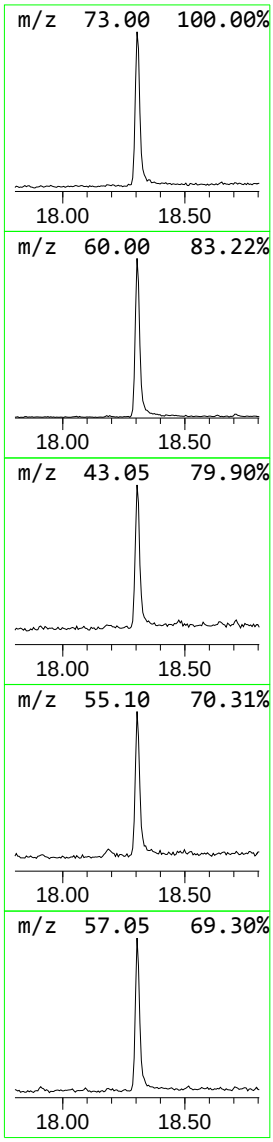
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.304	6.23 ng/ul	1020470	Phenanthrene-d10	17.445

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	99
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tridecanoic acid	214	C13H26O2	000638-53-9	91





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Data File : BP014155.D
Acq On : 20 Mar 2023 23:36
Operator : CG/JU
Sample : 01885-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB907

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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

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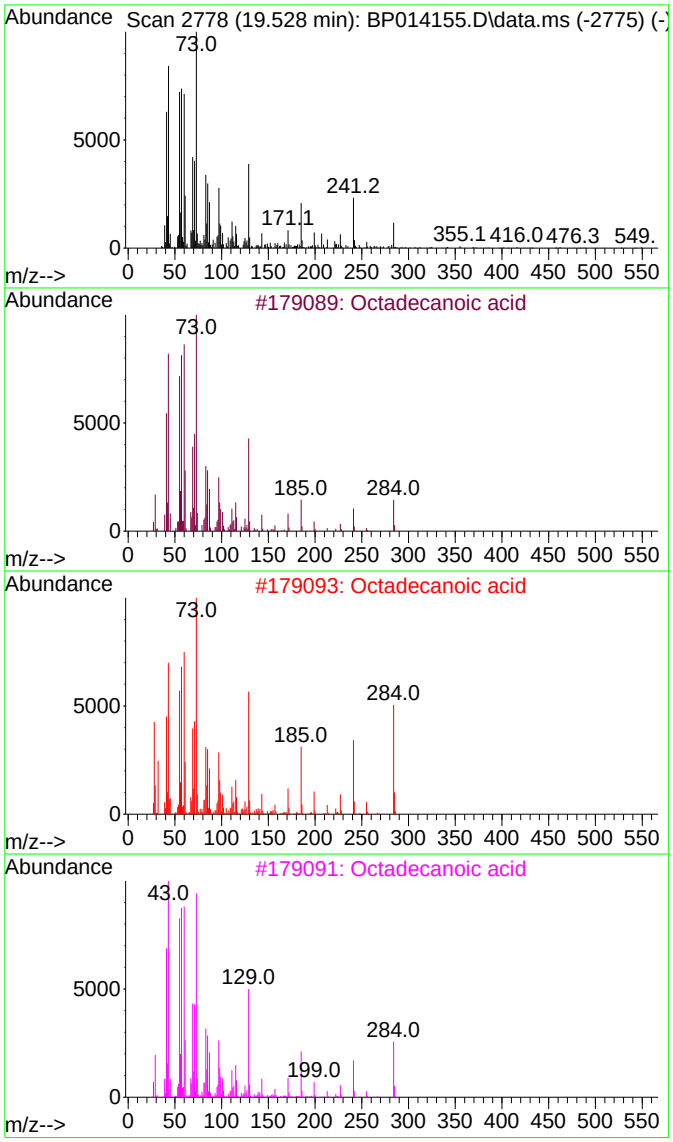
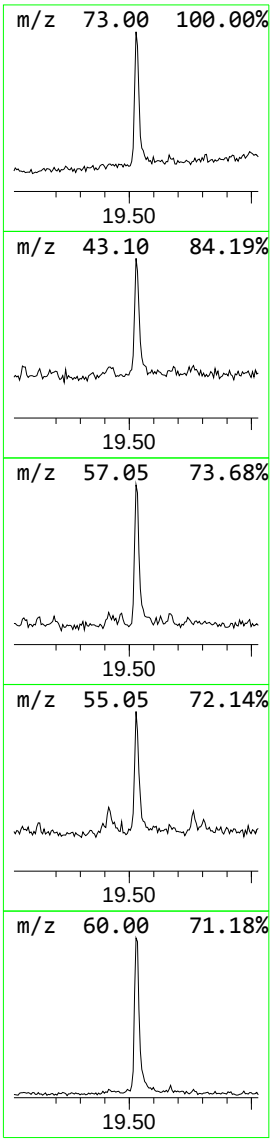
Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.528	2.43 ng/ul	410304	Chrysene-d12	21.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





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Data File : BP014155.D
Acq On : 20 Mar 2023 23:36
Operator : CG/JU
Sample : 01885-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB907

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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

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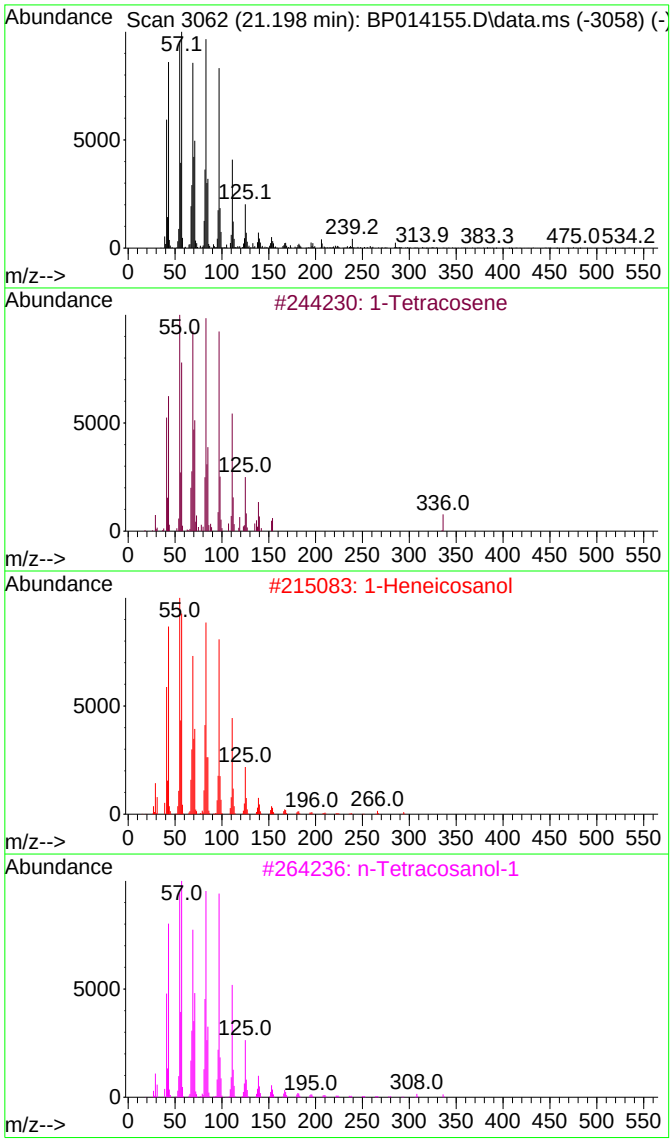
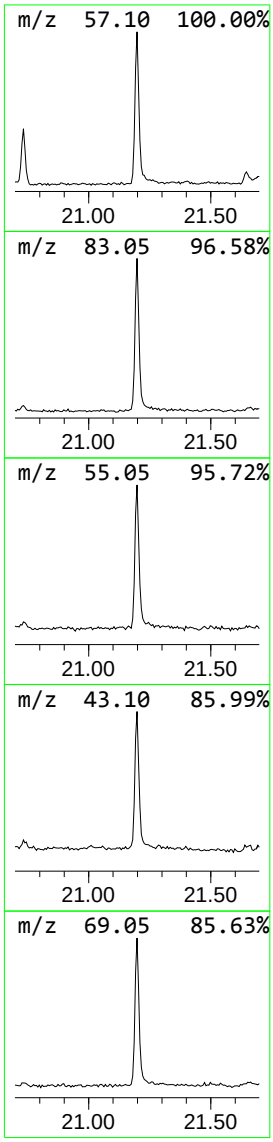
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.198	5.60 ng/ul	942922	Chrysene-d12	21.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032023\
Data File : BP014155.D
Acq On : 20 Mar 2023 23:36
Operator : CG/JU
Sample : 01885-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB907

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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

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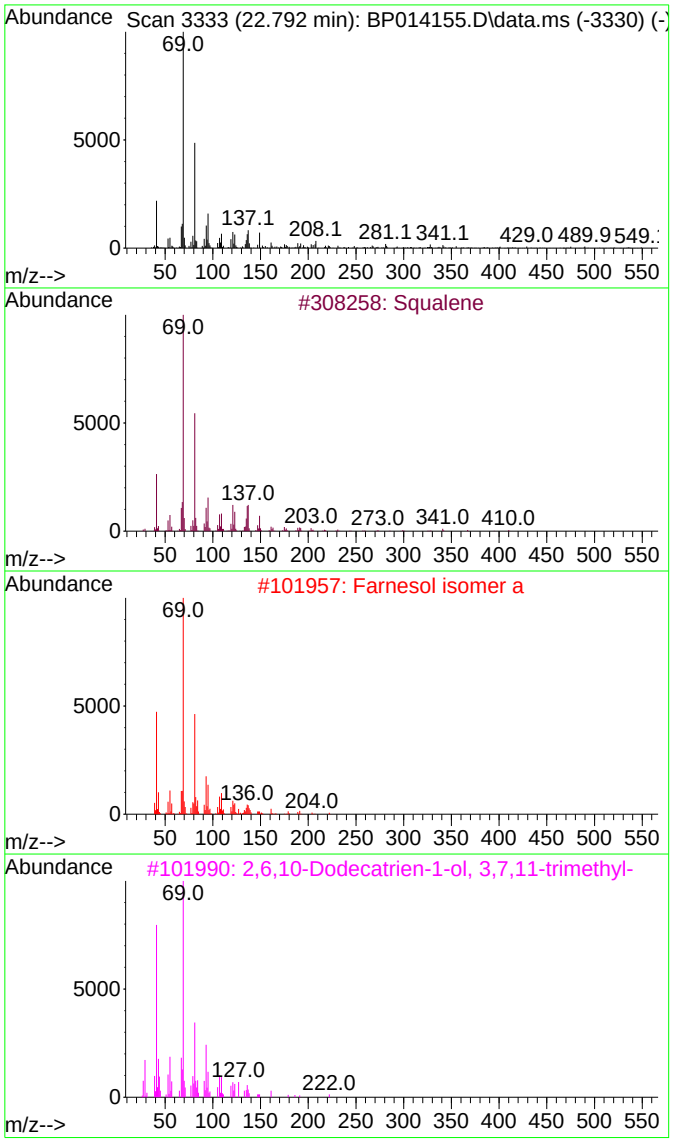
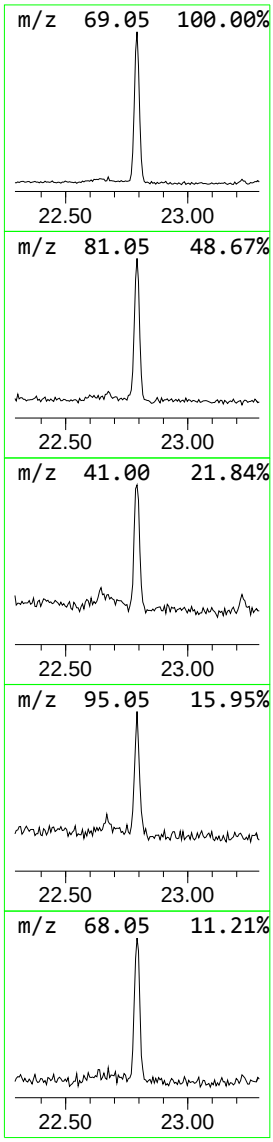
Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.792	2.40 ng/ul	344584	Perylene-d12	24.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	72
2	Farnesol isomer a	222	C15H26O	1000108-92-4	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
4	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	64
5	Supraene	410	C30H50	007683-64-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032023\
Data File : BP014155.D
Acq On : 20 Mar 2023 23:36
Operator : CG/JU
Sample : 01885-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB907

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3-Oxathiolane	4.634	2.0	ng/ul	132580	1	8.052	1298440	20.0
Phenol, p-tert-...	12.204	2.5	ng/ul	235606	2	10.875	1901020	20.0
Benzenesulfonam...	16.204	21.5	ng/ul	3520210	4	17.445	3278380	20.0
Benzenesulfonam...	16.716	12.8	ng/ul	2103420	4	17.445	3278380	20.0
n-Hexadecanoic ...	18.304	6.2	ng/ul	1020470	4	17.445	3278380	20.0
Octadecanoic acid	19.528	2.4	ng/ul	410304	5	21.528	3370540	20.0
(DEL) Alkane: S...	21.198	5.6	ng/ul	942922	5	21.528	3370540	20.0
Squalene	22.792	2.4	ng/ul	344584	6	24.045	2869340	20.0