LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

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_M\Methods\SFAM-EPA-BM040922.M
Title : SVOA CALIBRATION

Signal : TIC: BM034678.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.243	32	35	45	rVB2	30209	42326	2.22%	0.165%
2	3.672	105	108	116	rBV	269627	425012	22.33%	1.660%
3	4.013	161	166	175	rVB3	36235	58154	3.05%	0.227%
4	4.231	199	203	212	rVB5	23859	36795	1.93%	0.144%
5	4.849	305	308	314	rVB5	11681	17330	0.91%	0.068%
6	5.031	336	339	344	rVB5	8273	12325	0.65%	0.048%
7	5.154	355	360	369	rVB	43916	69620	3.66%	0.272%
8	5.296	381	384	393	rBV4	16499	30508	1.60%	0.119%
9	5.737	456	459	465	rVB7	6143	9814	0.52%	0.038%
10	5.943	490	494	499	rVB2	23450	34319	1.80%	0.134%
11	6.125	522	525	531	rVB2	11817	16800	0.88%	0.066%
12	6.537	591	595	601	rVB6	7116	12134	0.64%	0.047%
13	6.760	630	633	640	rVB	8987	12243	0.64%	0.048%
14	6.854	642	649	654	rBV4	12252	30314	1.59%	0.118%
15	6.948	663	665	670	rVB2	5410	7316	0.38%	0.029%
16	7.025	672	678	690	rBV	334720	628477	33.01%	2.455%
17	7.190	701	706	715	rBV	300010	475725	24.99%	1.858%
18	7.395	731	741	755	rVB	367743	663754	34.87%	2.593%
19	7.866	814	821	830	rBV	441222	731636	38.43%	2.858%
20	7.937	830	833	839	rVB3	13973	22304	1.17%	0.087%
21	8.084	854	858	865	rVV9	6691	11009	0.58%	0.043%
22	8.160	866	871	880	rVB	51261	88141	4.63%	0.344%
23	8.342	897	902	905	rBV6	5160	11348	0.60%	0.044%
24	8.431	916	917	923	rVB6	5305	8122	0.43%	0.032%
25	8.578	936	942	962	rBV	421526	779011	40.92%	3.043%
26	9.025	1008	1018	1032	rBV	353180	701731	36.86%	2.741%
27	9.142	1033	1038	1045	rVB	23719	52249	2.74%	0.204%
28	9.242	1051	1055	1062	rVB2	18683	32703	1.72%	0.128%
29	9.372	1072	1077	1082	rVB8	8438	16448	0.86%	0.064%
30	9.466	1089	1093	1098	rVV3	14080	23806	1.25%	0.093%
31	9.566	1106	1110	1115	rVB6	4205	6474	0.34%	0.025%
32	9.684	1125	1130	1135	rBV5	13330	23318	1.22%	0.091%
33	9.754	1135	1142	1150	rBV	276612	499831	26.26%	1.952%
34	10.178	1209	1214	1221	rBV8	4916	9412	0.49%	0.037%
35	10.295	1227	1234	1251	rBV	394100	740278	38.89%	2.891%
36	10.672	1291	1298	1313	rVB	609001	1014581	53.29%	3.963%

LSC Area Percent Report

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Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

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_M\Methods\SFAM-EPA-BM040922.M
Title : SVOA CALIBRATION

37	10.813	1314	1322	1332	rBV	319268	653687	34.34%	2.553%
38	10.901	1332	1337	1349	rVB4	45117	102793	5.40%	0.401%
39	11.130	1367	1376	1383	rBV10	16520	40243	2.11%	0.157%
40	11.219	1387	1391	1396	rVB4	23920	38513	2.02%	0.150%
41	11.630	1447	1461	1473	rBV	107446	260514	13.68%	1.018%
42	11.725	1473	1477	1488	rVV3	27763	68239	3.58%	0.267%
43	11.819	1488	1493	1500	rVV2	19633	44082	2.32%	0.172%
44	11.883	1500	1504	1512	rVV8	10253	23981	1.26%	0.094%
45	12.036	1526	1530	1536	rVV7	11484	25712	1.35%	0.100%
46	12.101	1536	1541	1549	rVV3	43285	105610	5.55%	0.413%
47	12.183	1549	1555	1566	rVV	42416	113000	5.94%	0.441%
48	12.266	1566	1569	1577	rVB5	9279	16541	0.87%	0.065%
49	12.389	1584	1590	1602	rVB	140153	223292	11.73%	0.872%
50	12.560	1614	1619	1624	rVB6	4187	8702	0.46%	0.034%
51	12.783	1652	1657	1664	rVB8	4493	9132	0.48%	0.036%
52	12.930	1676	1682	1685	rBV6	8609	17678	0.93%	0.069%
53	13.060	1702	1704	1708	rVB5	5039	5975	0.31%	0.023%
54	13.248	1727	1736	1742	rBV9	17864	46726	2.45%	0.183%
55	13.348	1747	1753	1761	rVB2	28809	41156	2.16%	0.161%
56	13.442	1764	1769	1775	rBV	79141	125156	6.57%	0.489%
57	13.572	1785	1791	1797	rBV2	33654	56946	2.99%	0.222%
58	13.919	1844	1850	1862	rBV	758619	1146421	60.22%	4.478%
59	14.001	1862	1864	1869	rVV4	8381	10649	0.56%	0.042%
60	14.060	1869	1874	1878	rVB6	6012	10814	0.57%	0.042%
61	14.207	1888	1899	1910	rBV	861571	1326851	69.70%	5.183%
62	14.307	1913	1916	1919	rVV4	6299	9755	0.51%	0.038%
63	14.336	1919	1921	1926	rVB6	4507	6165	0.32%	0.024%
64	14.419	1931	1935	1937	rBV3	10118	11813	0.62%	0.046%
65	14.460	1937	1942	1945	rVV5	15938	28341	1.49%	0.111%
66	14.513	1945	1951	1958	rVB	870532	1242702	65.28%	4.854%
67	14.718	1979	1986	2002	rBV2	77228	262973	13.81%	1.027%
68	15.148	2056	2059	2062	rVV4	5906	9061	0.48%	0.035%
69	15.177	2062	2064	2068	rVB5	6197	6172	0.32%	0.024%
70	15.289	2078	2083	2094	rBV	89280	226146	11.88%	0.883%
71	15.501	2113	2119	2131	rBV	1119984	1650762	86.71%	6.448%
72	15.624	2134	2140	2154	rVV	308162	487771	25.62%	1.905%
73	15.748	2157	2161	2164	rVB5	9006	14707	0.77%	0.057%
74	16.177	2230	2234	2238	rBV7	6689	11496	0.60%	0.045%
75	16.224	2240	2242	2245	rVV3	7871	9253	0.49%	0.036%
76	16.248	2245	2246	2249	rVV3	5785	5607	0.29%	0.022%

LSC Area Percent Report

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Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ETNQ3

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_M\Methods\SFAM-EPA-BM040922.M
Title : SVOA CALIBRATION

77	16.289	2249	2253	2256	rVV6	3893	6105	0.32%	0.024%
78	16.330	2256	2260	2269	rVV5	23152	40886	2.15%	0.160%
79	16.407	2269	2273	2278	rVB7	5662	11104	0.58%	0.043%
80	16.483	2281	2286	2293	rBV8	13651	28871	1.52%	0.113%
81	16.542	2293	2296	2302	rBV8	3055	5503	0.29%	0.021%
82	16.683	2318	2320	2325	rVB5	6330	8678	0.46%	0.034%
83	17.030	2374	2379	2381	rBV5	4871	8624	0.45%	0.034%
84	17.254	2411	2417	2428	rBV	1002134	1423591	74.78%	5.560%
85	17.354	2428	2434	2449	rVV	1114283	1663886	87.40%	6.499%
86	17.936	2529	2533	2537	rBV2	25918	33982	1.79%	0.133%
87	18.154	2566	2570	2576	rBV3	33039	57256	3.01%	0.224%
88	19.171	2739	2743	2746	rBV5	6223	9424	0.50%	0.037%
89	19.212	2746	2750	2754	rBV5	14240	21364	1.12%	0.083%
90	19.283	2758	2762	2767	rBV4	15042	26397	1.39%	0.103%
91	19.571	2807	2811	2815	rVB2	23675	32107	1.69%	0.125%
92	19.642	2818	2823	2829	rBV	1393906	1903715	100.00%	7.436%
93	19.689	2829	2831	2838	rVB	63482	96781	5.08%	0.378%
94	19.783	2845	2847	2852	rVB5	9495	11602	0.61%	0.045%
95	19.883	2861	2864	2869	rVB4	27647	33601	1.77%	0.131%
96	20.295	2930	2934	2938	rVB	40909	51046	2.68%	0.199%
97	21.142	3075	3078	3086	rBV2	66080	99997	5.25%	0.391%
98	21.430	3123	3127	3133	rBV	775560	1209349	63.53%	4.724%
99	23.653	3499	3505	3511	rBV2	747849	1524906	80.10%	5.956%
100	23.806	3525	3531	3543	rVB2	686213	1433013	75.27%	5.597%

Sum of corrected areas: 25602293

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
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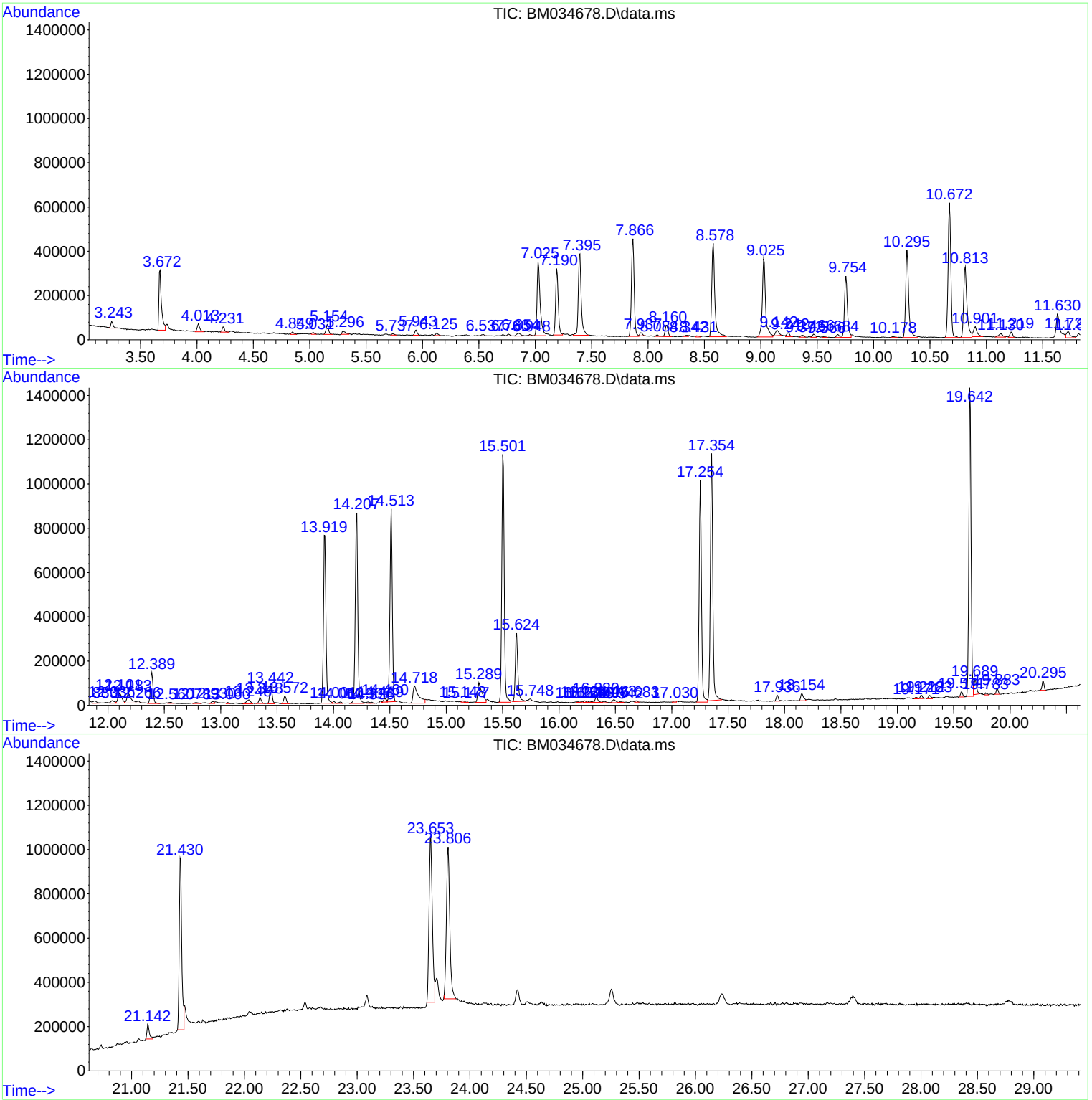
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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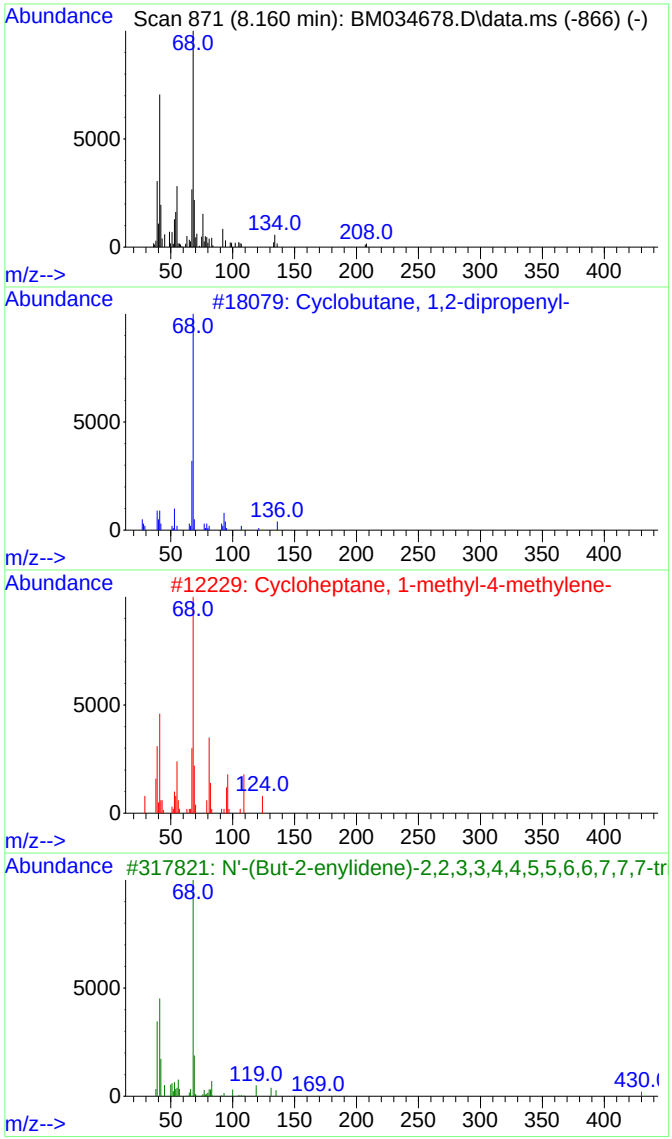
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

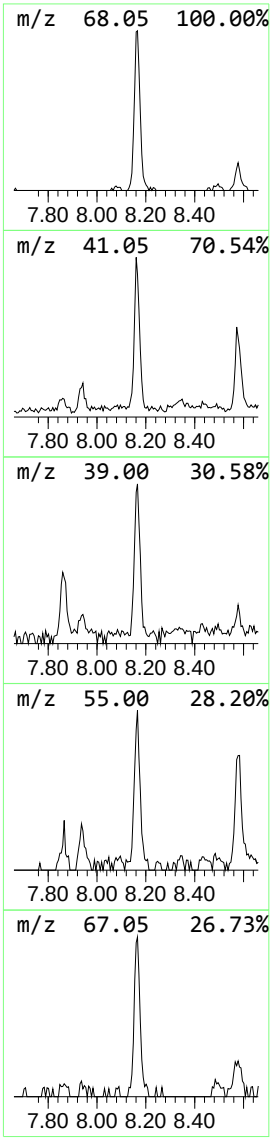
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclobutane, 1,2-dipropenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.160	2.41 ng/ul	88141	1,4-Dichlorobenzene-d4	7.866

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, 1,2-dipropenyl-	136	C10H16	022769-00-2	50
2	Cycloheptane, 1-methyl-4-methylene-	124	C9H16	023799-25-9	40
3	N'-(But-2-enylidene)-2,2,3,3,4,4...	430	C11H7F13N2O	330591-15-6	40
4	Tetrahydrocyclopenta[1,3]dioxin-...	142	C7H10O3	124898-85-7	40
5	Glutaric acid, di(3-methylbut-3-...	268	C15H24O4	1000359-95-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

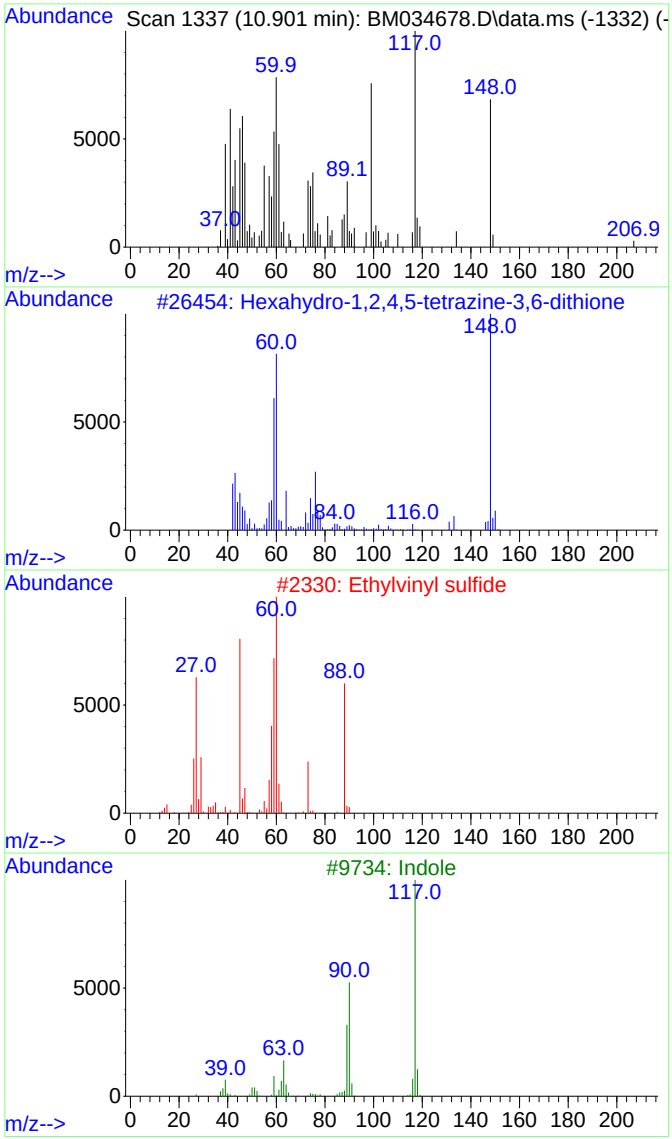
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

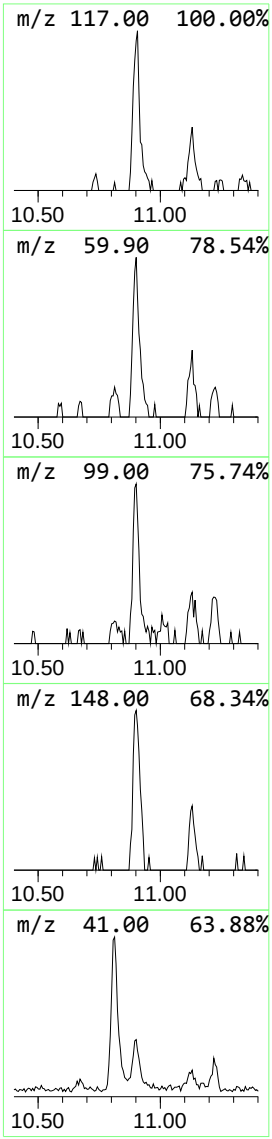
****

Peak Number 2 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.901	2.03 ng/ul	102793	Naphthalene-d8	10.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexahydro-1,2,4,5-tetrazine-3,6-...	148	C2H4N4S2	036239-33-5	22
2	Ethylvinyl sulfide	88	C4H8S	000627-50-9	14
3	Indole	117	C8H7N	000120-72-9	11
4	1,3-Dithiane, 2,2-dimethyl-	148	C6H12S2	006007-22-3	11
5	Thiirane	60	C2H4S	000420-12-2	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
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ALS Vial : 20 Sample Multiplier: 1

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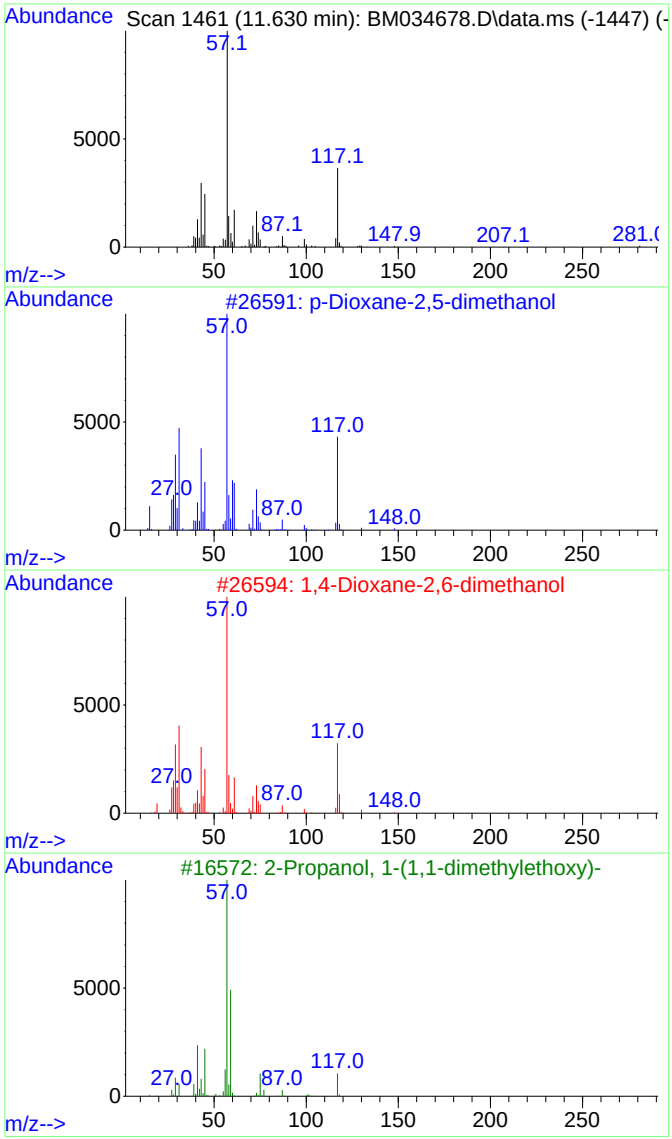
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

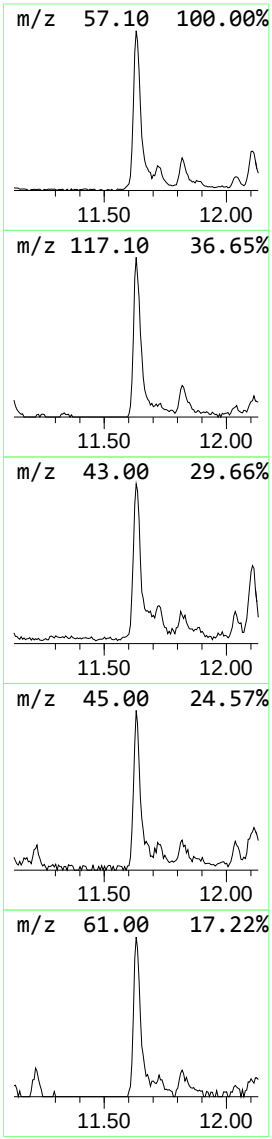
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 p-Dioxane-2,5-dimethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.631	5.14 ng/ul	260514	Naphthalene-d8	10.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Dioxane-2,5-dimethanol	148	C6H12O4	014236-12-5	87
2	1,4-Dioxane-2,6-dimethanol	148	C6H12O4	054120-69-3	72
3	2-Propanol, 1-(1,1-dimethylethoxy)-	132	C7H16O2	057018-52-7	38
4	3-Ethylheptanoic acid	158	C9H18O2	014272-47-0	32
5	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	25





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Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

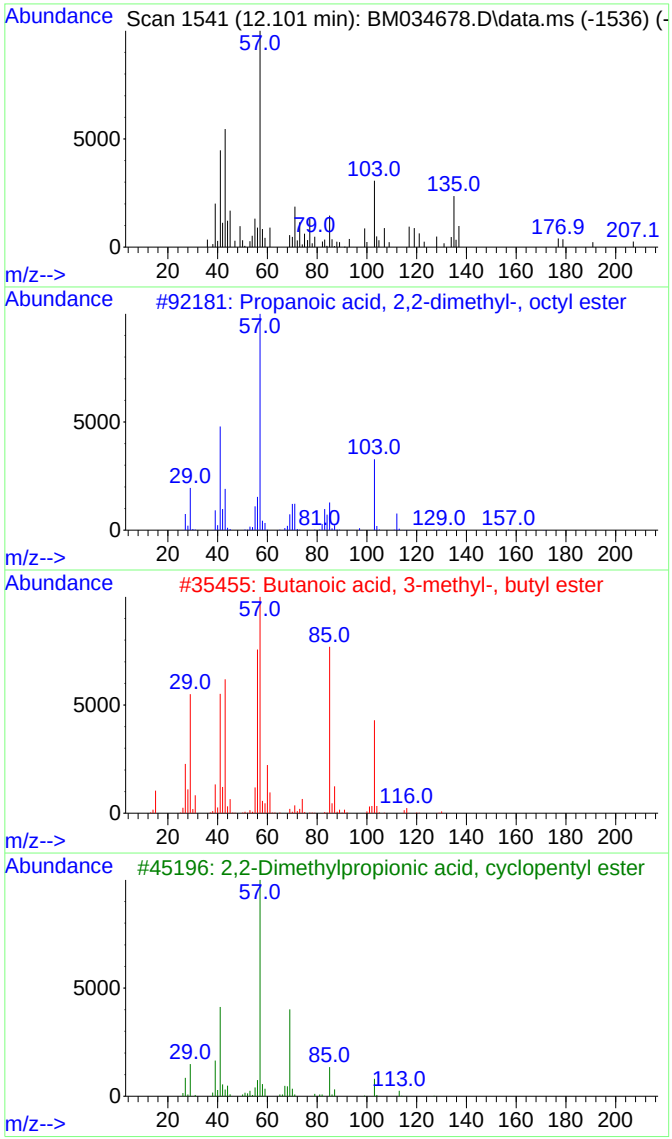
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

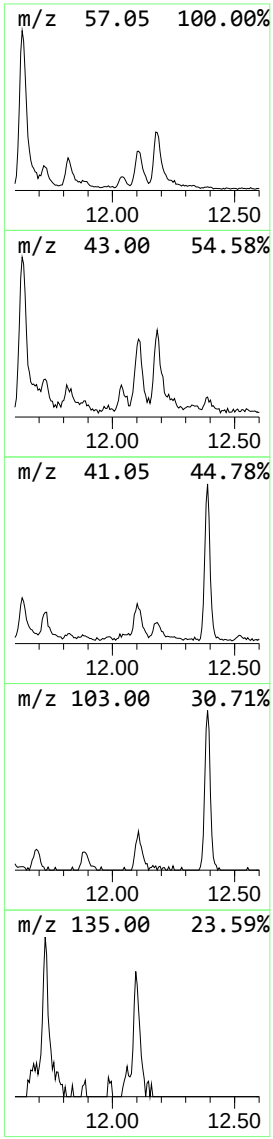
****

Peak Number 4 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.101	2.08 ng/ul	105610	Naphthalene-d8	10.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	27
2	Butanoic acid, 3-methyl-, butyl ...	158	C9H18O2	000109-19-3	16
3	2,2-Dimethylpropionic acid, cycl...	170	C10H18O2	1000278-99-9	16
4	3-Hexanone, 2,4-dimethyl-	128	C8H16O	018641-70-8	11
5	2-Butanone, 1-bromo-3,3-dimethyl-	178	C6H11BrO	005469-26-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

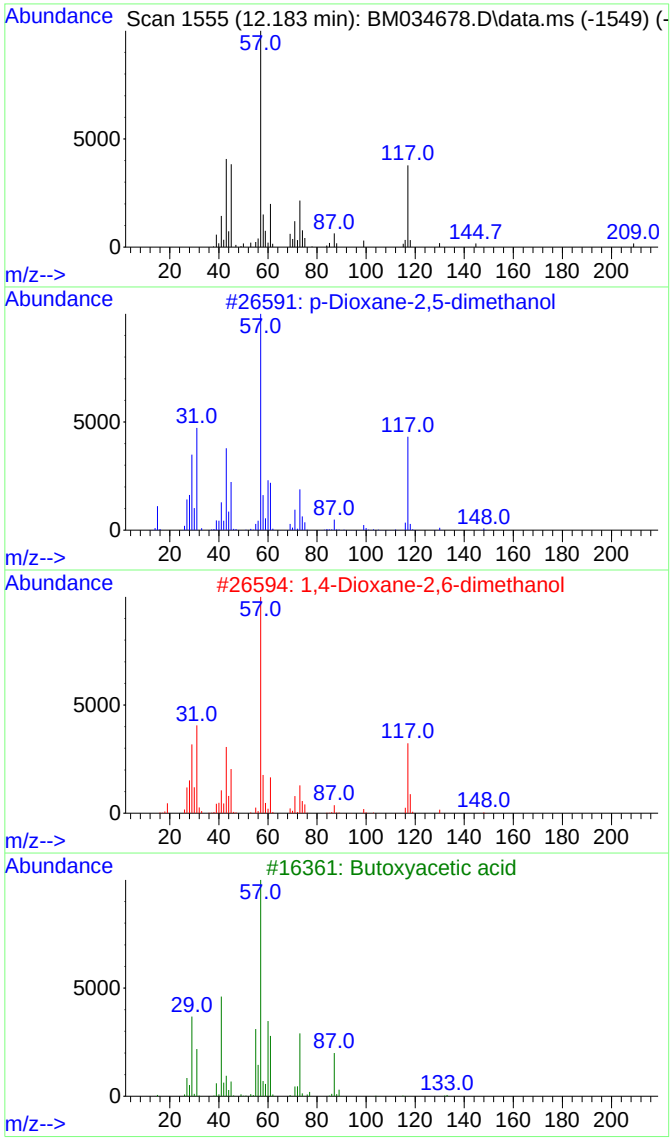
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

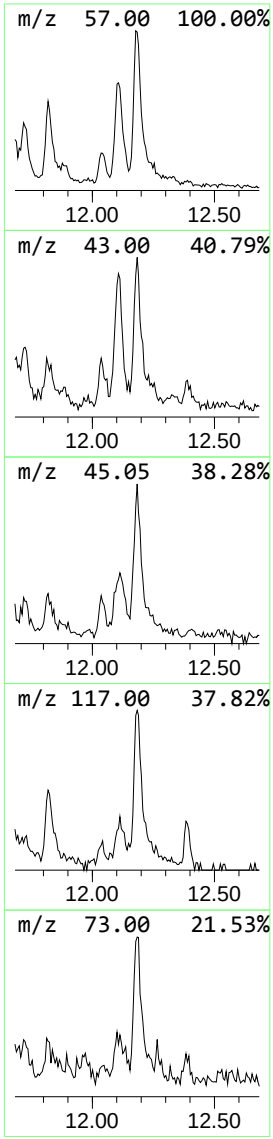
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4-Dioxane-2,6-dimethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.183	2.23 ng/ul	113000	Naphthalene-d8	10.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Dioxane-2,5-dimethanol	148	C6H12O4	014236-12-5	72
2	1,4-Dioxane-2,6-dimethanol	148	C6H12O4	054120-69-3	50
3	Butoxyacetic acid	132	C6H12O3	002516-93-0	38
4	3-Buten-2-ol	72	C4H8O	000598-32-3	35
5	Isobutyl pentan-2-yl carbonate	188	C10H20O3	1010372-76-8	23





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Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

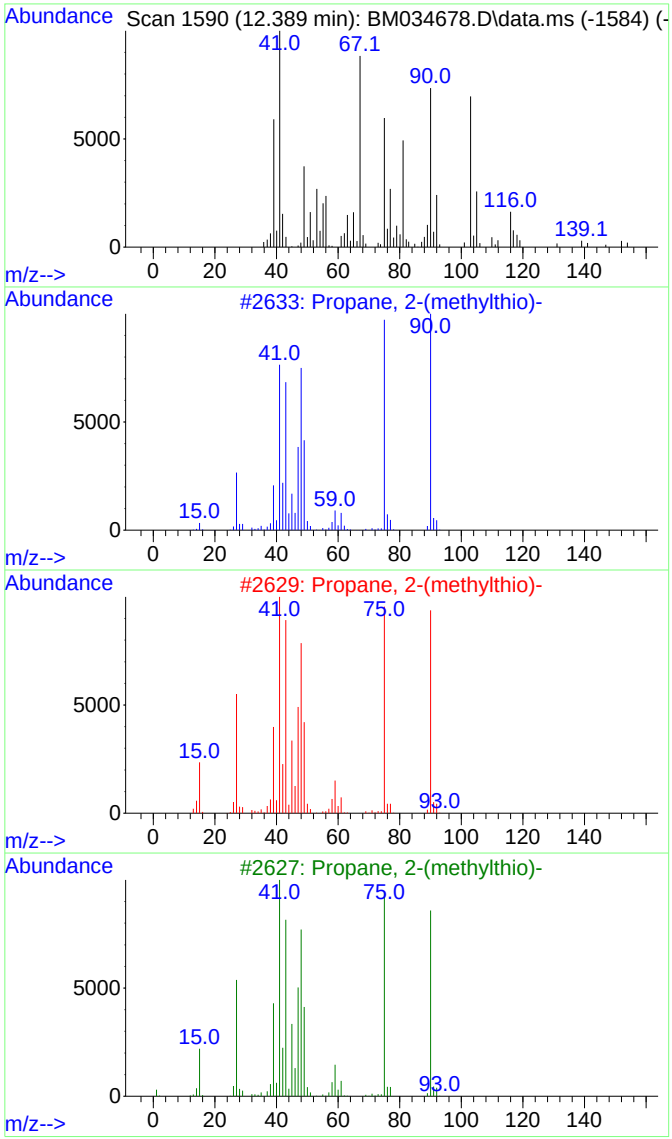
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

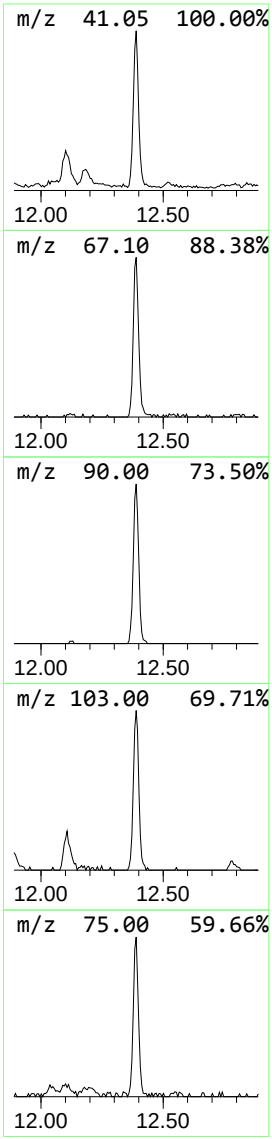
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propane, 2-(methylthio)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.389	4.40 ng/ul	223292	Naphthalene-d8	10.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	58
2	Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	50
3	Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	50
4	Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	47
5	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

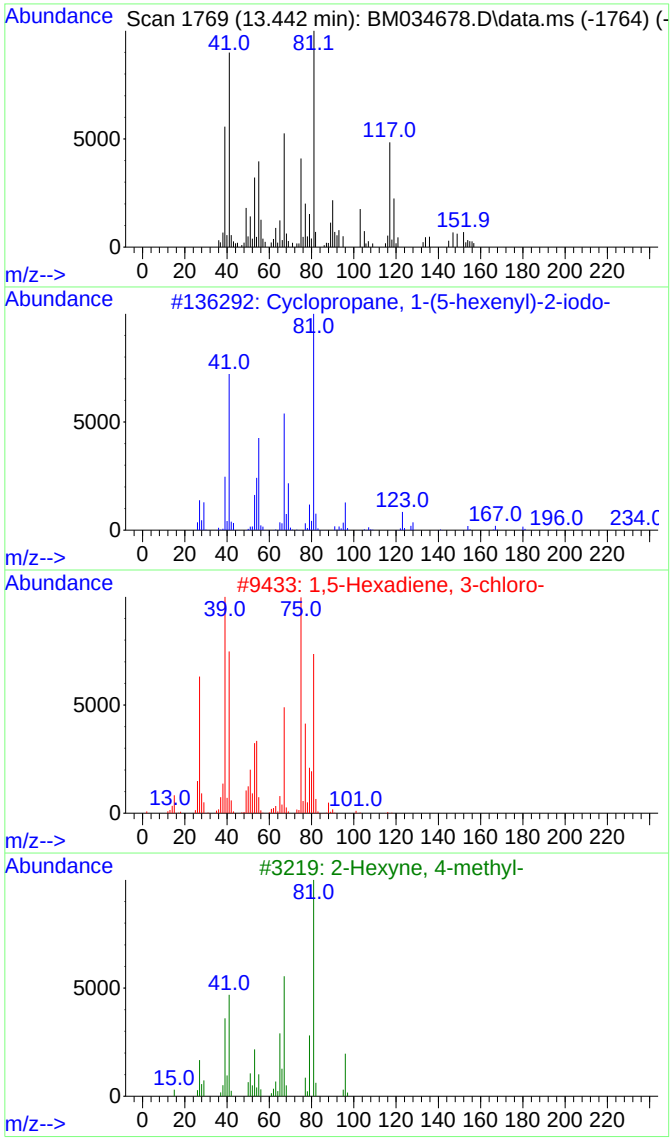
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

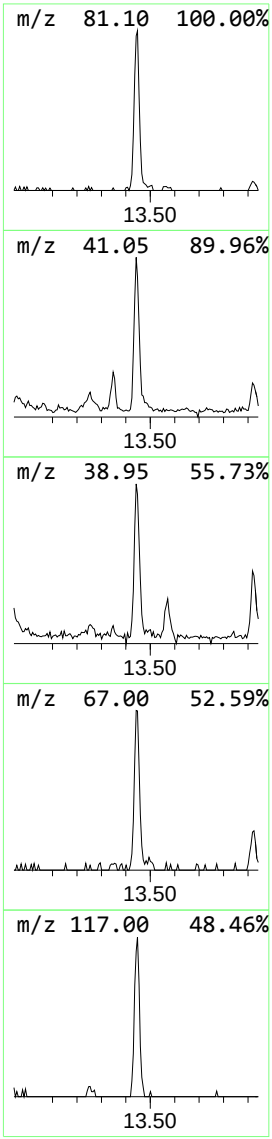
****

Peak Number 7 unknown-03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.442	2.01 ng/ul	125156	Acenaphthene-d10	14.513

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	27
2	1,5-Hexadiene, 3-chloro-	116	C6H9Cl	028374-86-9	16
3	2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	16
4	Cyclohexane, 1,3-dichloro-, cis-	152	C6H10Cl2	024955-63-3	16
5	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	16





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Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

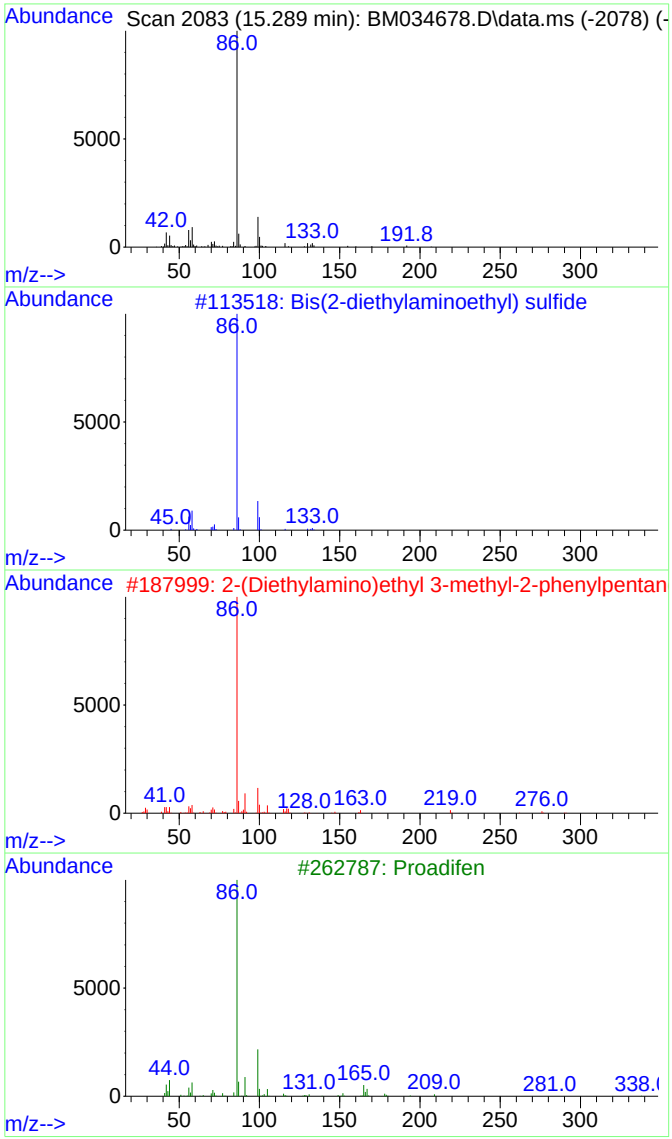
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.M
Quant Title : SVOA CALIBRATION

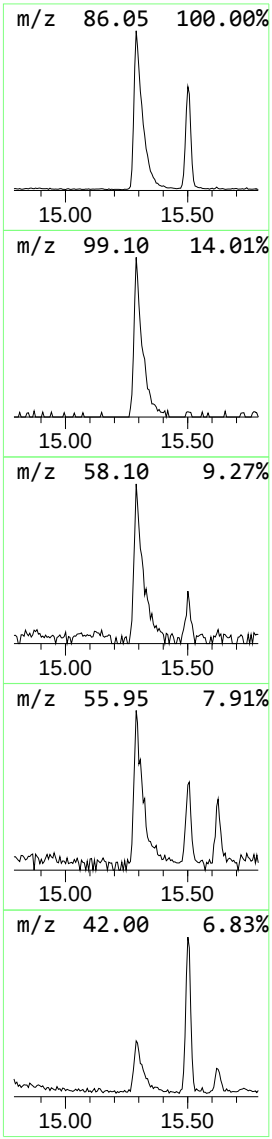
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bis(2-diethylaminoethyl) su... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.289	3.64 ng/ul	226146	Acenaphthene-d10	14.513

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-diethylaminoethyl) sulfide	232	C12H28N2S	006006-58-2	78
2	2-(Diethylamino)ethyl 3-methyl-2...	291	C18H29NO2	026878-41-1	72
3	Proadifen	353	C23H31NO2	000302-33-0	72
4	2-(Diethylamino)ethyl cyclohexyl...	333	C20H31NO3	003570-96-5	72
5	Cyclopentanecarboxylic acid, 1-p...	289	C18H27NO2	000077-22-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041422\
Data File : BM034678.D
Acq On : 14 Apr 2022 21:38
Operator : CG/JU
Sample : N2316-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETNQ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM040922.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
Cyclobutane, 1,...	8.160	2.4	ng/ul	88141	1	7.866	731636	20.0
unknown-01	10.901	2.0	ng/ul	102793	2	10.672	1014580	20.0
p-Dioxane-2,5-d...	11.631	5.1	ng/ul	260514	2	10.672	1014580	20.0
unknown-02	12.101	2.1	ng/ul	105610	2	10.672	1014580	20.0
1,4-Dioxane-2,6...	12.183	2.2	ng/ul	113000	2	10.672	1014580	20.0
Propane, 2-(met...	12.389	4.4	ng/ul	223292	2	10.672	1014580	20.0
unknown-03	13.442	2.0	ng/ul	125156	3	14.513	1242700	20.0
Bis(2-diethylam...	15.289	3.6	ng/ul	226146	3	14.513	1242700	20.0