LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041823\
Data File : BM039480.D
Acq On : 19 Apr 2023 05:17
Operator : CG/JU
Sample : 02335-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0MH8

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-BM041823.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM039480.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.216	3	5	14	rVB	57502	72285	0.90%	0.100%
2	3.652	76	79	93	rBV	117126	212488	2.65%	0.293%
3	3.969	130	133	140	rVB2	19359	28094	0.35%	0.039%
4	5.351	365	368	372	rBV	8289	9939	0.12%	0.014%
5	5.869	452	456	464	rVB5	7618	14281	0.18%	0.020%
6	6.934	631	637	641	rBV7	9089	20676	0.26%	0.029%
7	6.987	642	646	647	rVV3	8596	12198	0.15%	0.017%
8	7.022	647	652	664	rVB	140782	295481	3.69%	0.408%
9	7.163	670	676	694	rBV	949099	1567182	19.57%	2.164%
10	7.363	703	710	730	rBV	831949	1439153	17.97%	1.987%
11	7.828	782	789	797	rBV	766948	1289799	16.10%	1.781%
12	7.898	797	801	817	rVB	75860	158776	1.98%	0.219%
13	8.128	837	840	847	rVB7	6530	11698	0.15%	0.016%
14	8.469	892	898	902	rBV2	8571	17723	0.22%	0.024%
15	8.563	907	914	928	rBV	568098	1092279	13.64%	1.508%
16	8.663	928	931	938	rVB	24471	46430	0.58%	0.064%
17	8.939	971	978	983	rBV	199722	348876	4.36%	0.482%
18	8.998	983	988	996	rVV	1076838	1822709	22.76%	2.517%
19	9.163	1012	1016	1023	rVB7	12590	26302	0.33%	0.036%
20	9.392	1049	1055	1061	rBV	10506	18540	0.23%	0.026%
21	9.722	1104	1111	1128	rBV	896077	1650801	20.61%	2.279%
22	10.045	1161	1166	1171	rBV9	5036	10976	0.14%	0.015%
23	10.269	1197	1204	1227	rBV	1111556	2202442	27.50%	3.041%
24	10.551	1246	1252	1260	rBV	88559	172054	2.15%	0.238%
25	10.639	1260	1267	1274	rVV	1132065	2011714	25.12%	2.778%
26	10.698	1274	1277	1283	rVB	53908	83165	1.04%	0.115%
27	10.786	1285	1292	1313	rBV	908440	1889920	23.59%	2.610%
28	11.316	1375	1382	1390	rBV2	9013	20808	0.26%	0.029%
29	11.480	1403	1410	1411	rBV5	18932	32980	0.41%	0.046%
30	11.822	1461	1468	1475	rBV	21592	43425	0.54%	0.060%
31	11.886	1475	1479	1485	rVB2	9213	15605	0.19%	0.022%
32	11.963	1485	1492	1505	rBV	130712	321117	4.01%	0.443%
33	12.239	1532	1539	1545	rBV3	20411	42613	0.53%	0.059%
34	12.833	1636	1640	1649	rBV9	4447	11439	0.14%	0.016%
35	13.086	1678	1683	1690	rVB5	6957	14162	0.18%	0.020%
36	13.421	1729	1740	1761	rBV	664470	1258466	15.71%	1.738%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_M
ClientSampleId :
C0MH8

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-BM041823.MA.M
Title : SVOA CALIBRATION

37	13.569	1761	1765	1780	rVB5	17637	52399	0.65%	0.072%
38	13.904	1811	1822	1835	rBV	3015576	4355041	54.37%	6.013%
39	14.180	1861	1869	1884	rBV	3393182	5004383	62.48%	6.910%
40	14.292	1884	1888	1891	rVV2	5620	9706	0.12%	0.013%
41	14.368	1897	1901	1911	rVB3	16249	37740	0.47%	0.052%
42	14.486	1914	1921	1931	rVV	1981095	2914474	36.39%	4.024%
43	14.568	1931	1935	1942	rVB	42933	59838	0.75%	0.083%
44	14.757	1959	1967	1980	rBV5	37108	167735	2.09%	0.232%
45	14.904	1987	1992	1995	rVB7	5057	8175	0.10%	0.011%
46	15.163	2028	2036	2049	rVB	56514	117266	1.46%	0.162%
47	15.304	2051	2060	2066	rVB4	12655	34456	0.43%	0.048%
48	15.480	2081	2090	2107	rBV	4188483	6236764	77.86%	8.612%
49	15.615	2107	2113	2127	rVV	1384688	2162785	27.00%	2.986%
50	15.721	2127	2131	2136	rVV5	28919	58020	0.72%	0.080%
51	15.763	2136	2138	2143	rVB6	8057	11521	0.14%	0.016%
52	15.851	2149	2153	2158	rVB	40544	57086	0.71%	0.079%
53	16.057	2182	2188	2192	rBV6	17258	28947	0.36%	0.040%
54	16.104	2192	2196	2199	rVV6	5859	9287	0.12%	0.013%
55	16.827	2316	2319	2323	rVB2	8545	10943	0.14%	0.015%
56	17.239	2382	2389	2399	rVV	2365345	3408543	42.55%	4.706%
57	17.339	2399	2406	2431	rVV	4715365	7003102	87.43%	9.670%
58	17.521	2434	2437	2442	rVB	14063	19427	0.24%	0.027%
59	17.839	2485	2491	2495	rBV8	9824	21356	0.27%	0.029%
60	17.904	2497	2502	2517	rVV	820414	1080793	13.49%	1.492%
61	18.074	2528	2531	2536	rVB4	13973	18598	0.23%	0.026%
62	18.139	2538	2542	2550	rBV2	43712	93256	1.16%	0.129%
63	18.209	2550	2554	2556	rBV	15540	18896	0.24%	0.026%
64	18.351	2575	2578	2582	rBV4	11621	14033	0.18%	0.019%
65	18.386	2582	2584	2589	rVB4	18700	23405	0.29%	0.032%
66	18.639	2623	2627	2630	rBV5	9263	14084	0.18%	0.019%
67	18.715	2637	2640	2644	rVB4	8109	9023	0.11%	0.012%
68	19.198	2718	2722	2729	rBV	59513	87059	1.09%	0.120%
69	19.274	2730	2735	2741	rBV	52439	86848	1.08%	0.120%
70	19.415	2756	2759	2767	rBV3	45369	96001	1.20%	0.133%
71	19.556	2781	2783	2787	rBV4	12619	12417	0.16%	0.017%
72	19.633	2790	2796	2817	rBV	5628652	8010002	100.00%	11.060%
73	19.868	2833	2836	2843	rBV7	21217	32763	0.41%	0.045%
74	20.645	2964	2968	2977	rBV2	170468	283554	3.54%	0.392%
75	21.427	3096	3101	3116	rBV	2415722	3316076	41.40%	4.579%
76	23.644	3471	3478	3495	rVB2	3104594	6327429	78.99%	8.737%

LSC Area Percent Report

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Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MH8

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Title : SVOA CALIBRATION

77	23.797	3497	3504	3517	rVB2	1347606	2822889	35.24%	3.898%

Sum of corrected areas: 72422716

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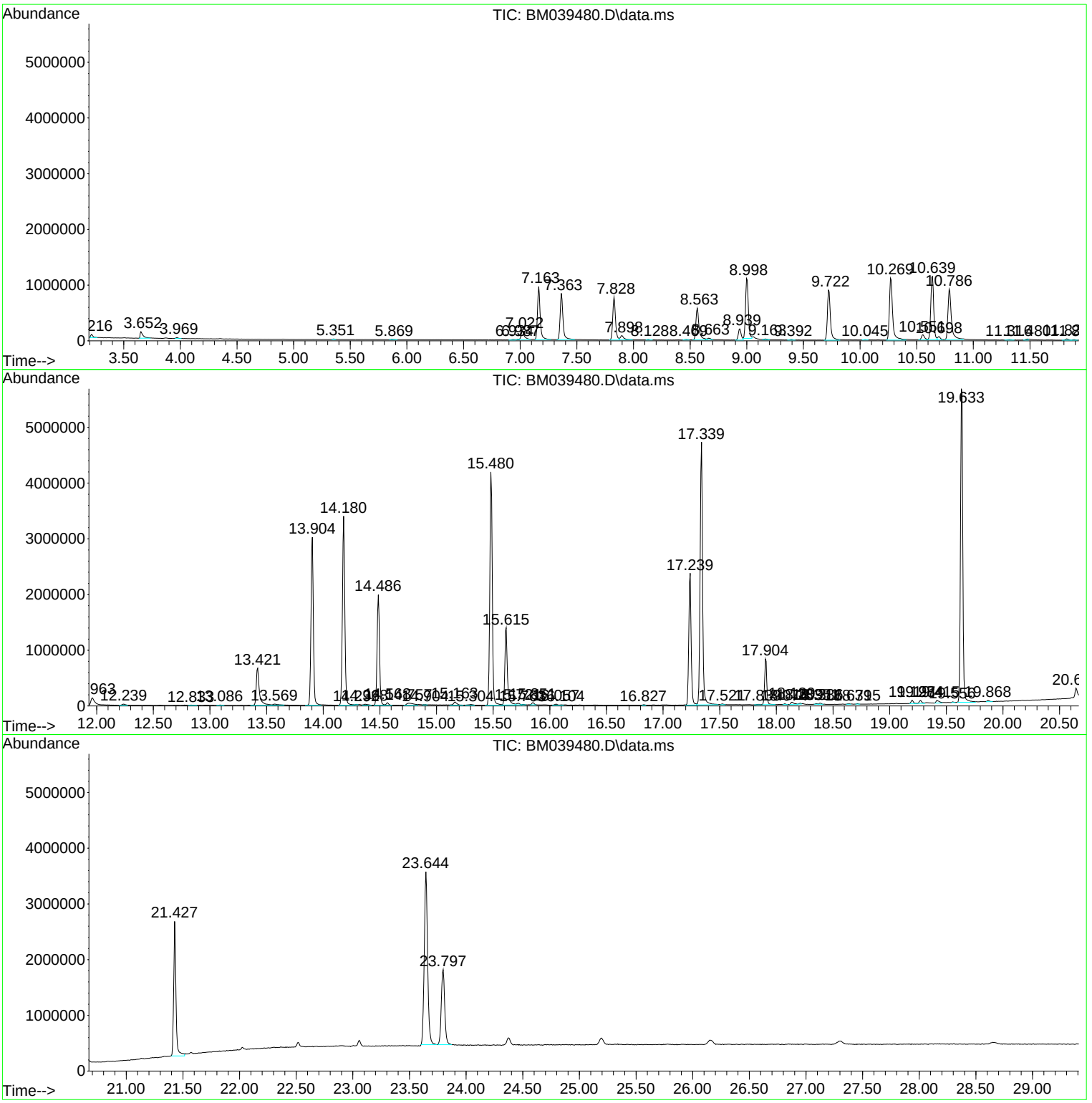
Operator : CG/JU
Sample : 02335-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041823\
Data File : BM039480.D
Acq On : 19 Apr 2023 05:17
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Instrument :
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ClientSampleId :
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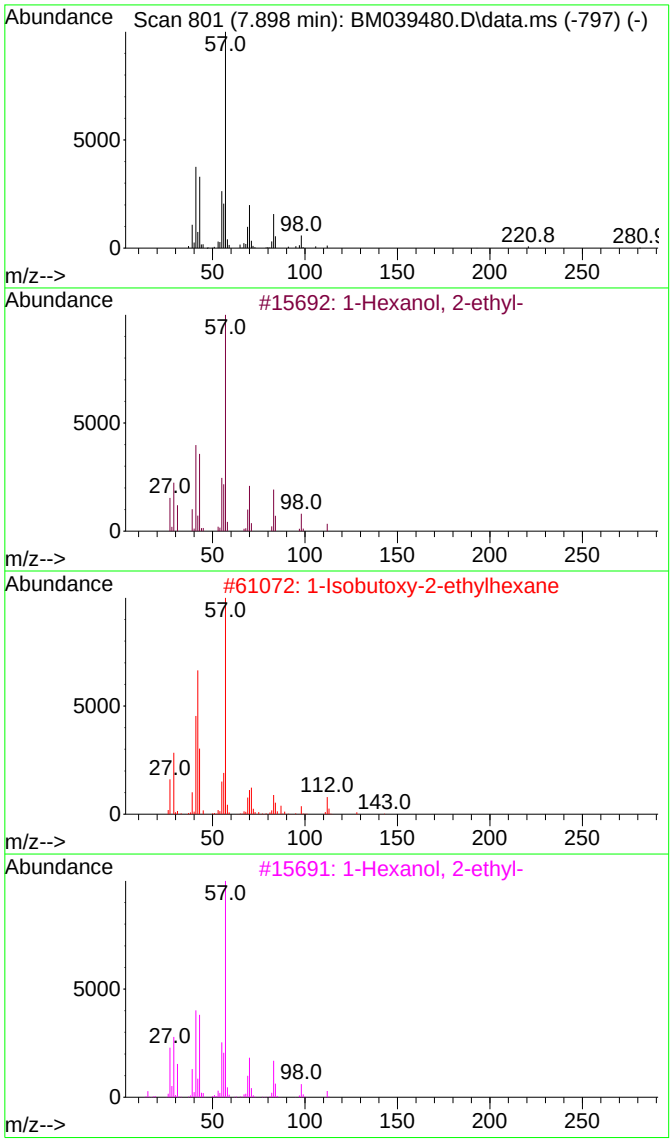
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

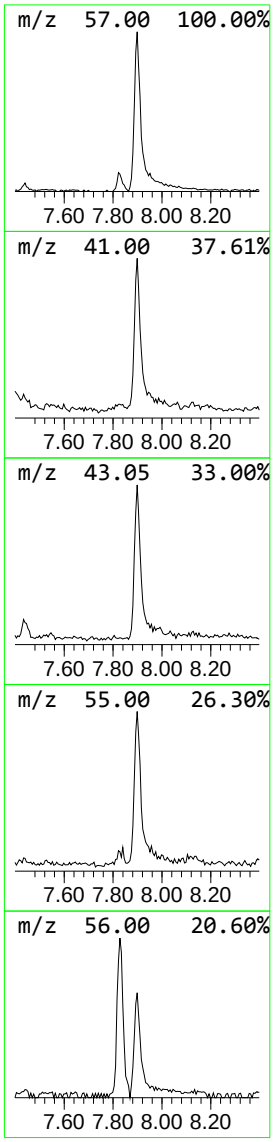
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	2.46 ng/ul	158776	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041823\
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Sample : 02335-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

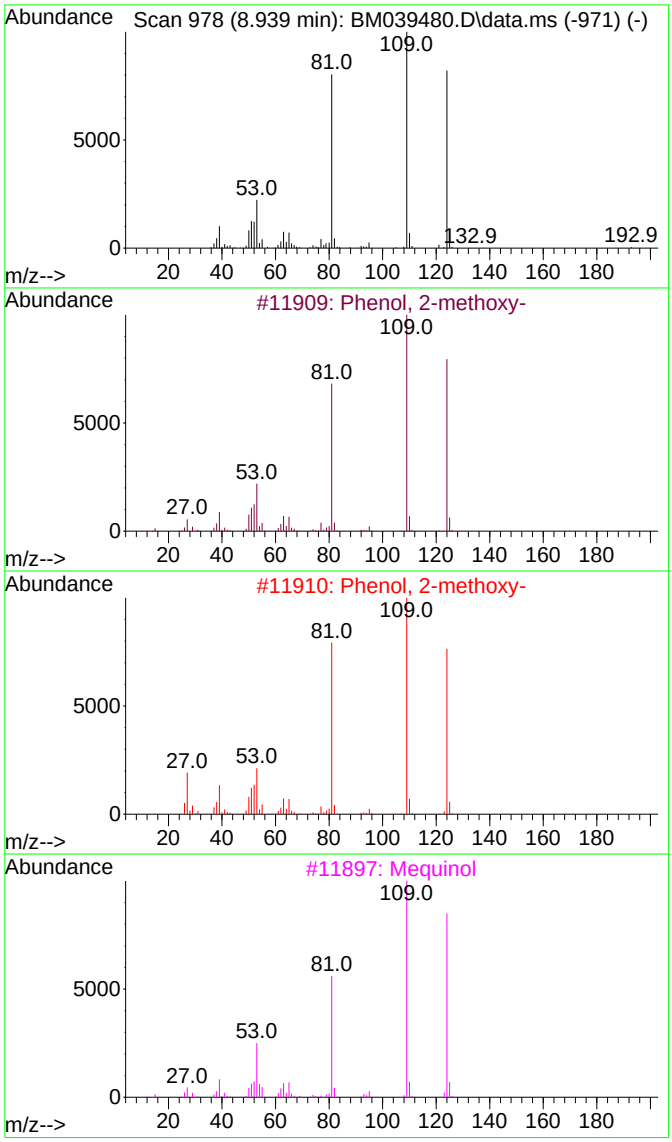
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

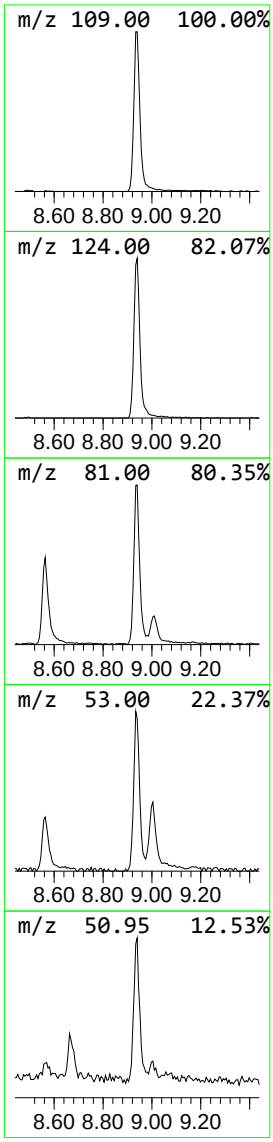
****

Peak Number 2 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.939	5.41 ng/ul	348876	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
3	Mequinol	124	C7H8O2	000150-76-5	91
4	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90
5	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041823\
Data File : BM039480.D
Acq On : 19 Apr 2023 05:17
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Sample : 02335-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

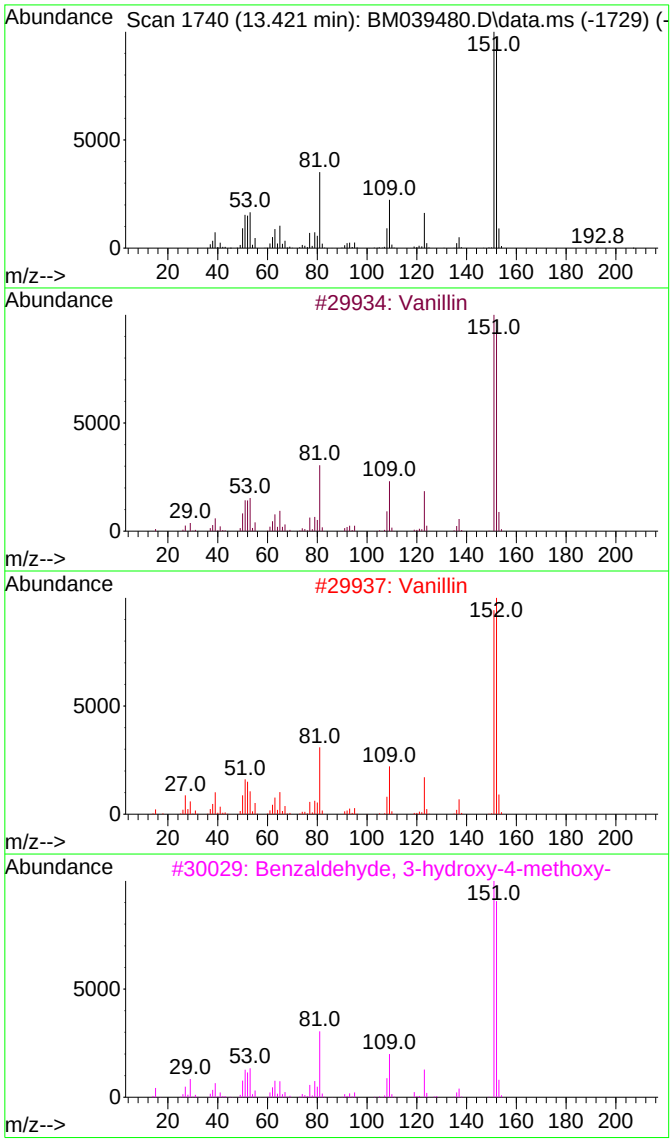
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

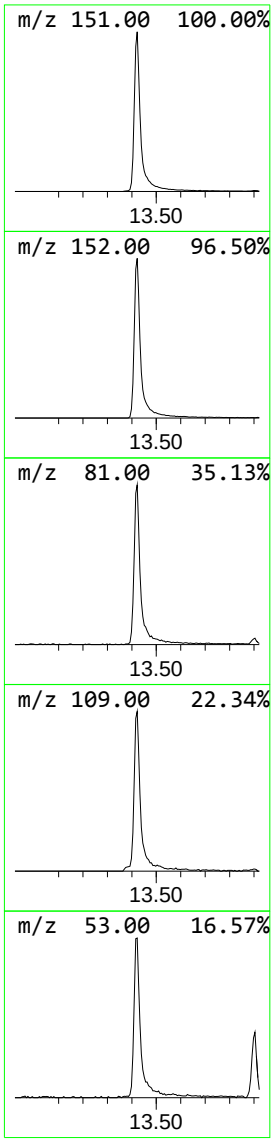
****

Peak Number 3 Vanillin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.422	8.64 ng/ul	1258470	Acenaphthene-d10	14.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	97
2	Vanillin	152	C8H8O3	000121-33-5	97
3	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
4	Vanillin	152	C8H8O3	000121-33-5	97
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96





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Instrument :
BNA_M
ClientSampleId :
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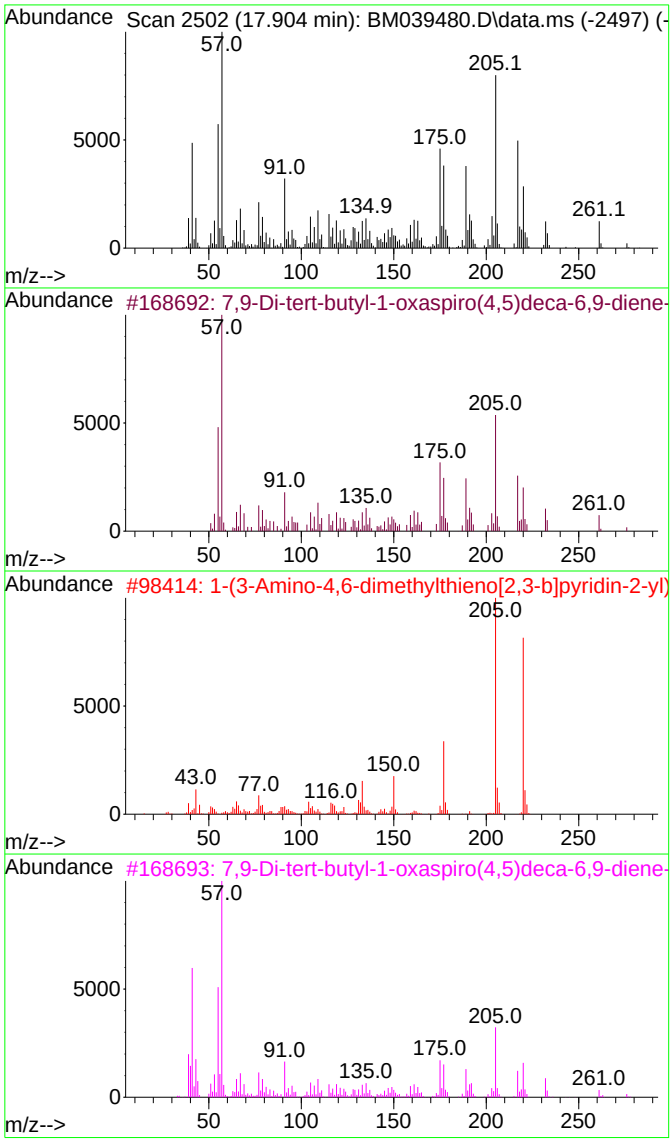
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

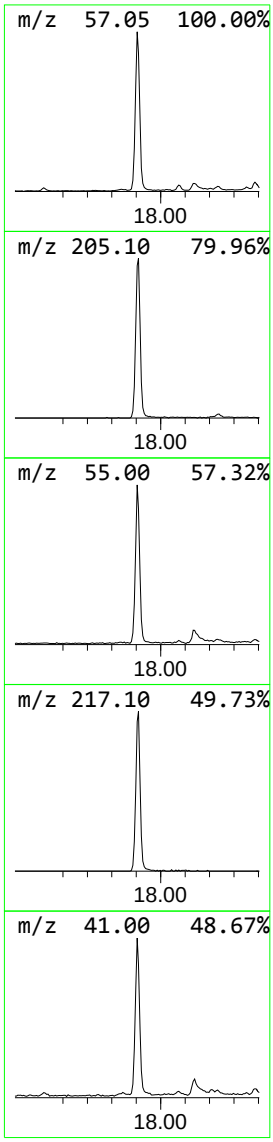
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.904	6.34 ng/ul	1080790	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	55
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	55
4	(Z)-((2-Benzylideneheptyl)oxy)tr...	276	C17H28OSi	1000495-65-9	51
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50





Tentatively Identified Compound (LSC) summary

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.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-Hexanol, 2-et...	7.898	2.5	ng/ul	158776	1	7.828	1289800	20.0
Phenol, 2-methoxy-	8.939	5.4	ng/ul	348876	1	7.828	1289800	20.0
Vanillin	13.422	8.6	ng/ul	1258470	3	14.486	2914470	20.0
7,9-Di-tert-but...	17.904	6.3	ng/ul	1080790	4	17.239	3408540	20.0