LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM091817\
Data File : BM011587.D
Acq On : 19 Sep 2017 02:04
Operator : SJ/JU
Sample : I5271-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC5

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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.393	14	18	27	rVB	146695	198862	1.55%	0.146%
2	4.040	124	128	136	rVB7	11852	23709	0.18%	0.017%
3	4.240	158	162	170	rVB5	14814	29428	0.23%	0.022%
4	4.510	203	208	213	rVB6	15134	24620	0.19%	0.018%
5	5.275	333	338	347	rBV	81638	132633	1.03%	0.097%
6	5.457	365	369	372	rBV3	15237	23021	0.18%	0.017%
7	5.498	373	376	382	rVB2	13216	21367	0.17%	0.016%
8	6.010	456	463	479	rBV	3324636	5151147	40.02%	3.774%
9	6.622	559	567	572	rBV4	19368	43129	0.34%	0.032%
10	6.939	615	621	629	rBV3	29912	76088	0.59%	0.056%
11	7.057	637	641	645	rBV4	27179	45937	0.36%	0.034%
12	7.116	645	651	667	rVB	435706	808593	6.28%	0.592%
13	7.245	667	673	675	rBV2	10532	17380	0.14%	0.013%
14	7.292	675	681	692	rBV	1609940	2486572	19.32%	1.822%
15	7.498	709	716	730	rBV	1479114	2481188	19.28%	1.818%
16	7.745	753	758	761	rBV6	10797	18282	0.14%	0.013%
17	7.857	773	777	782	rVB4	16197	28568	0.22%	0.021%
18	7.969	788	796	801	rBV	1752677	2910492	22.61%	2.132%
19	8.022	801	805	818	rVB	668872	1141128	8.87%	0.836%
20	8.251	842	844	849	rVV4	15668	22914	0.18%	0.017%
21	8.322	850	856	863	rVB	124174	215157	1.67%	0.158%
22	8.581	894	900	907	rBV3	39268	73771	0.57%	0.054%
23	8.663	907	914	925	rBV	1181143	1981201	15.39%	1.451%
24	8.792	931	936	949	rVB	55575	109807	0.85%	0.080%
25	9.063	975	982	988	rBV	868717	1456304	11.32%	1.067%
26	9.128	988	993	999	rVV	1870550	3258525	25.32%	2.387%
27	9.175	999	1001	1007	rVB	200798	291825	2.27%	0.214%
28	9.292	1014	1021	1030	rVB3	81672	174235	1.35%	0.128%
29	9.522	1054	1060	1064	rBV3	15346	22548	0.18%	0.017%
30	9.692	1084	1089	1097	rVB6	9616	19208	0.15%	0.014%
31	9.851	1107	1116	1131	rBV	1511018	2620365	20.36%	1.920%
32	9.998	1134	1141	1146	rVV6	21588	60928	0.47%	0.045%
33	10.069	1150	1153	1164	rVV7	19649	53971	0.42%	0.040%
34	10.186	1168	1173	1180	rBV9	8455	21186	0.16%	0.016%

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Misc :
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Instrument : BNA_M
ClientSampleId : C0AC5

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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Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Title : SVOA CALIBRATION

35	10.386	1200	1207	1223	rBV	2202913	3746835	29.11%	2.745%
36	10.674	1250	1256	1266	rVB	398830	723214	5.62%	0.530%
37	10.774	1266	1273	1279	rVV	2610989	4381362	34.04%	3.210%
38	10.822	1279	1281	1291	rVB2	104682	154948	1.20%	0.114%
39	10.910	1291	1296	1306	rBV2	63272	130519	1.01%	0.096%
40	11.010	1308	1313	1317	rVB3	18559	30180	0.23%	0.022%
41	11.069	1319	1323	1332	rVB10	12147	25422	0.20%	0.019%
42	11.157	1333	1338	1343	rVB5	16674	29151	0.23%	0.021%
43	11.310	1357	1364	1367	rBV6	8155	17642	0.14%	0.013%
44	11.380	1367	1376	1381	rVV8	9204	26330	0.20%	0.019%
45	11.433	1381	1385	1395	rVB5	26743	62703	0.49%	0.046%
46	11.545	1395	1404	1415	rBV10	25564	80778	0.63%	0.059%
47	11.757	1434	1440	1442	rBV6	21578	33603	0.26%	0.025%
48	11.933	1466	1470	1475	rBV2	53100	89541	0.70%	0.066%
49	12.039	1480	1488	1502	rBV	597062	1076566	8.36%	0.789%
50	12.263	1521	1526	1531	rBV5	12181	19031	0.15%	0.014%
51	12.357	1535	1542	1551	rVB2	53624	98853	0.77%	0.072%
52	12.657	1589	1593	1600	rBV	12510	22362	0.17%	0.016%
53	12.804	1612	1618	1623	rBV6	12623	21518	0.17%	0.016%
54	12.868	1623	1629	1638	rVV2	44651	91502	0.71%	0.067%
55	12.957	1638	1644	1652	rVB	71283	130333	1.01%	0.095%
56	13.057	1657	1661	1666	rVV2	17061	33771	0.26%	0.025%
57	13.198	1677	1685	1691	rBV	131409	202971	1.58%	0.149%
58	13.515	1728	1739	1765	rBV	2369513	3644679	28.32%	2.670%
59	13.998	1815	1821	1837	rVV	4642817	6672983	51.85%	4.889%
60	14.121	1837	1842	1848	rVB5	27040	40218	0.31%	0.029%
61	14.292	1865	1871	1882	rBV	5104300	7391968	57.44%	5.416%
62	14.457	1894	1899	1909	rVB	64244	122909	0.96%	0.090%
63	14.598	1916	1923	1932	rBV2	3765841	5840511	45.38%	4.279%
64	14.668	1932	1935	1942	rVB	45708	67549	0.52%	0.049%
65	14.786	1949	1955	1974	rBV	248101	543260	4.22%	0.398%
66	14.992	1986	1990	2000	rVB3	38277	68565	0.53%	0.050%
67	15.174	2018	2021	2028	rVB4	16405	23721	0.18%	0.017%
68	15.262	2028	2036	2041	rBV	98311	156291	1.21%	0.115%
69	15.398	2052	2059	2067	rVB4	54057	123977	0.96%	0.091%
70	15.586	2084	2091	2101	rBV	6828493	9798484	76.13%	7.179%
71	15.698	2103	2110	2122	rBV	2467038	3437934	26.71%	2.519%

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Instrument : BNA_M
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Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Title : SVOA CALIBRATION

72	15.827	2127	2132	2137	rVV2	74668	129571	1.01%	0.095%
73	15.874	2137	2140	2145	rVV5	15715	25921	0.20%	0.019%
74	15.951	2148	2153	2162	rVB	61892	112628	0.88%	0.083%
75	16.215	2195	2198	2204	rVB6	9152	18863	0.15%	0.014%
76	16.721	2277	2284	2290	rBV8	23959	56929	0.44%	0.042%
77	16.921	2313	2318	2321	rBV5	15474	23098	0.18%	0.017%
78	16.998	2328	2331	2337	rBV2	22673	32968	0.26%	0.024%
79	17.339	2382	2389	2399	rBV	4829532	6822923	53.01%	4.999%
80	17.439	2399	2406	2422	rVB	8299918	11493925	89.31%	8.421%
81	17.603	2430	2434	2441	rVB	46171	67312	0.52%	0.049%
82	17.992	2494	2500	2513	rBV	1320488	1696326	13.18%	1.243%
83	18.162	2525	2529	2532	rBV2	25071	33735	0.26%	0.025%
84	18.209	2532	2537	2547	rVV	676514	1032573	8.02%	0.756%
85	18.286	2547	2550	2562	rVB2	86417	202436	1.57%	0.148%
86	18.421	2570	2573	2577	rVV4	22801	26765	0.21%	0.020%
87	18.474	2577	2582	2591	rVB2	49878	73023	0.57%	0.053%
88	18.721	2620	2624	2627	rBV5	13268	22925	0.18%	0.017%
89	19.356	2727	2732	2740	rBV	79189	136838	1.06%	0.100%
90	19.480	2748	2753	2768	rBV	1481281	2231062	17.34%	1.635%
91	19.609	2771	2775	2785	rVV2	83477	198253	1.54%	0.145%
92	19.721	2788	2794	2806	rVV	9959473	12869992	100.00%	9.429%
93	20.727	2963	2965	2969	rVB	56146	54929	0.43%	0.040%
94	21.191	3041	3044	3048	rBV	112153	126832	0.99%	0.093%
95	21.503	3091	3097	3104	rBV	5427088	7036841	54.68%	5.155%
96	21.627	3115	3118	3123	rVB2	126281	150923	1.17%	0.111%
97	22.080	3193	3195	3199	rVB	131768	139186	1.08%	0.102%
98	22.574	3275	3279	3284	rBV	325814	455851	3.54%	0.334%
99	23.721	3466	3474	3490	rVB2	5183683	10267863	79.78%	7.523%
100	23.874	3493	3500	3510	rVB	2933528	5747658	44.66%	4.211%

Sum of corrected areas: 136494422

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Instrument : BNA_M
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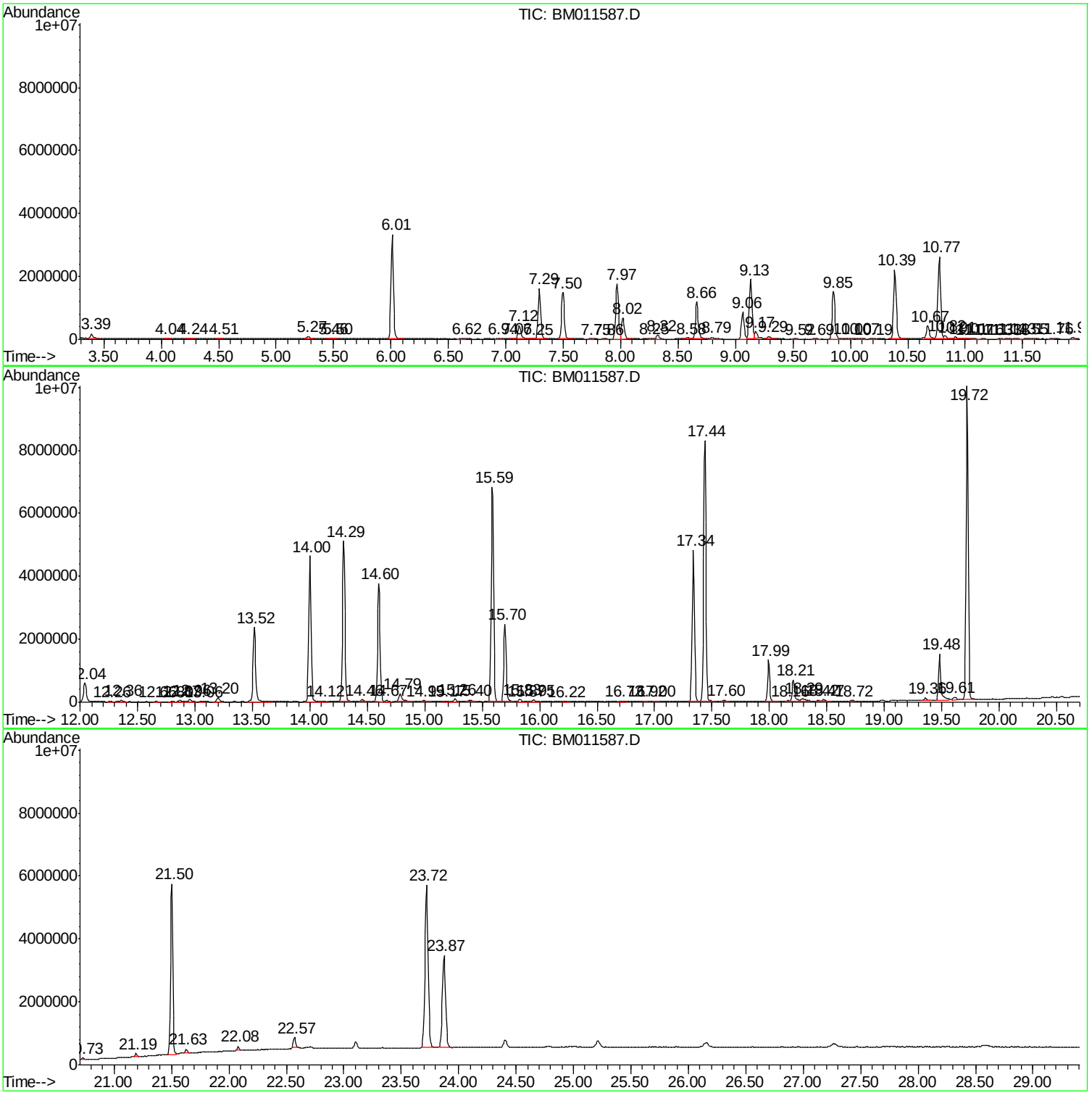
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Quant Title : SVOA CALIBRATION

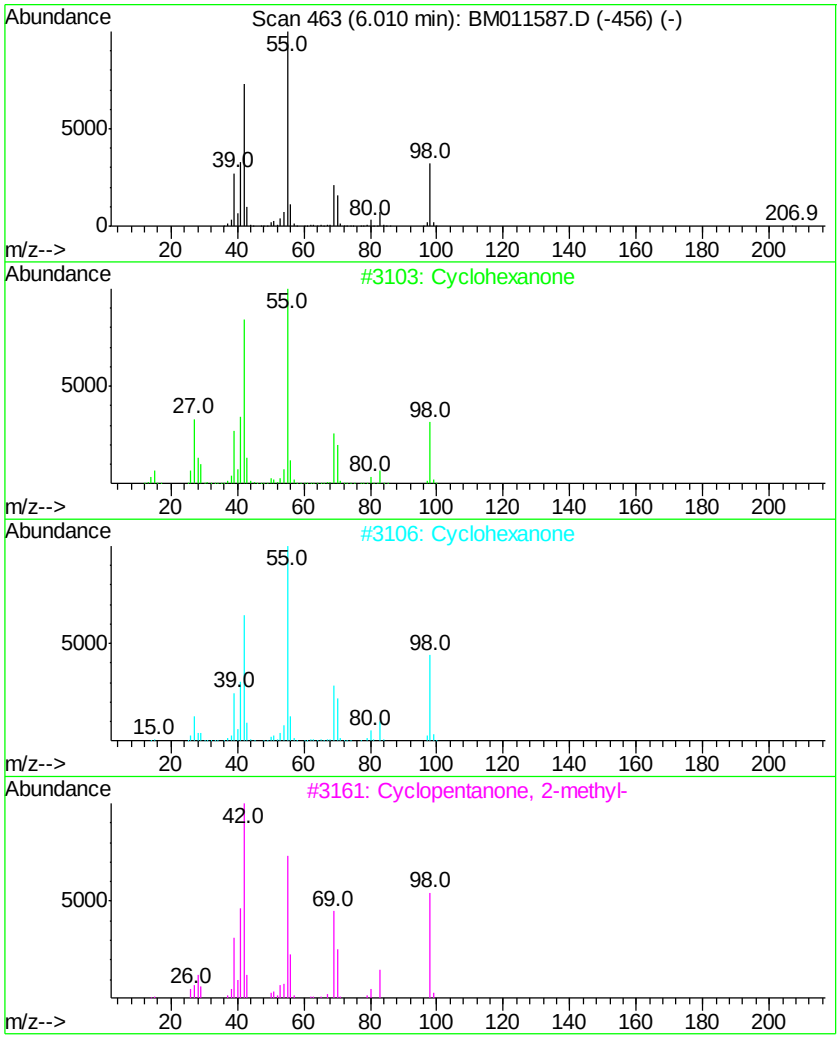
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

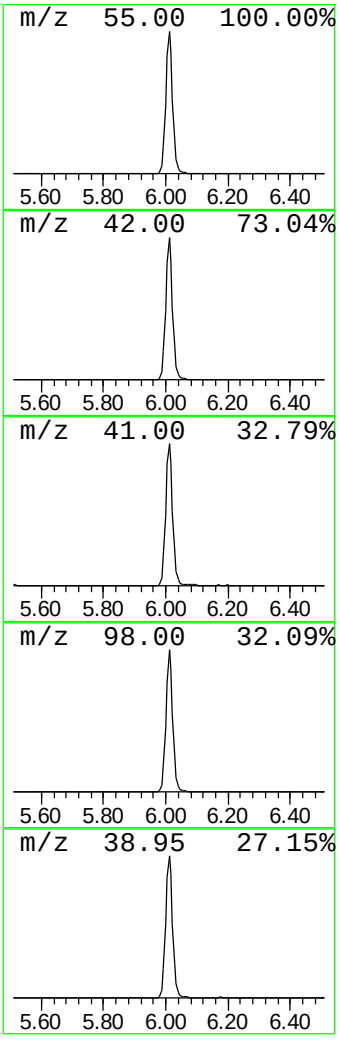
****

Peak Number 1 Cyclohexanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.01	35.40 ng/ul	5151150	1,4-Dichlorobenzene-d4	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	94
2	Cyclohexanone	98	C6H10O	000108-94-1	90
3	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	83
4	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	83
5	Cyclohexanone	98	C6H10O	000108-94-1	80





Library Search Compound Report

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Sample : I5271-01
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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

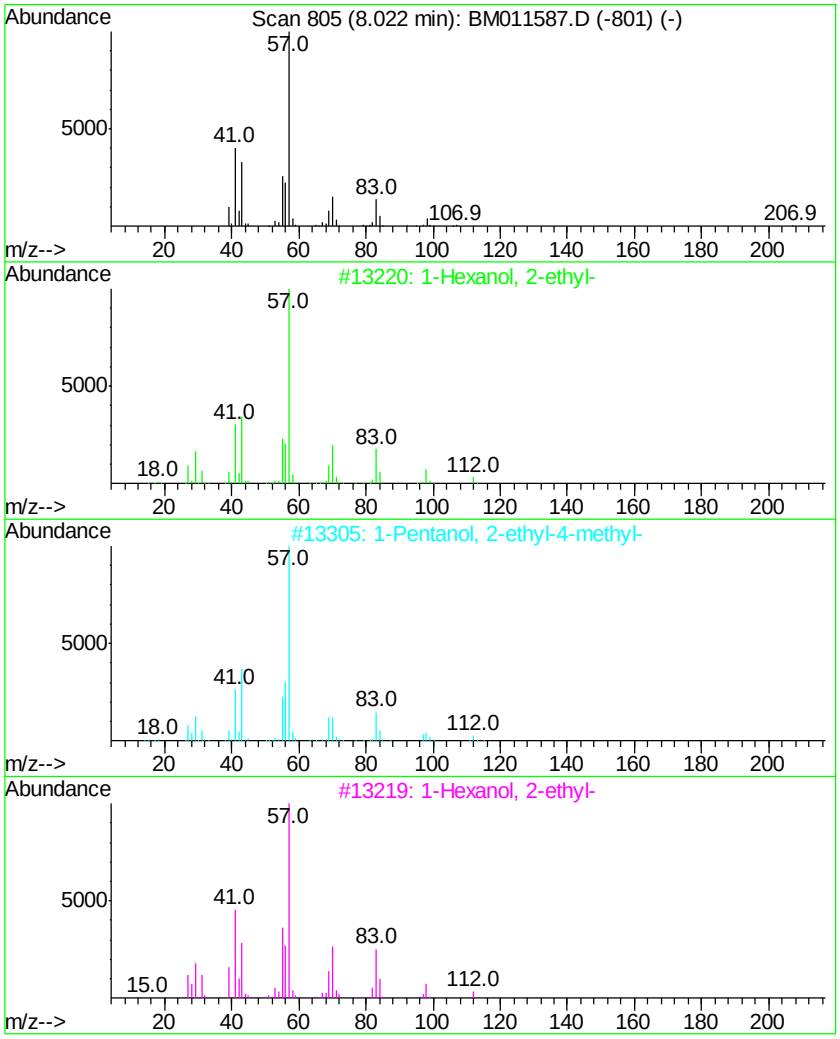
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

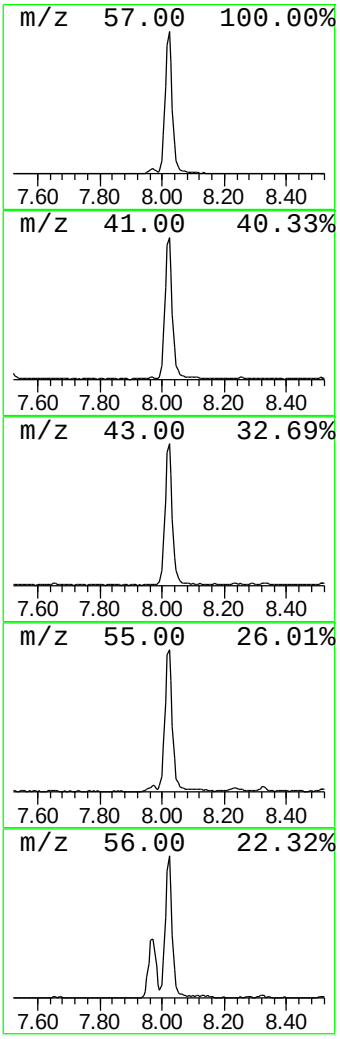
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.02	7.84 ng/ul	1141130	1,4-Dichlorobenzene-d4	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
4	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	50
5	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50





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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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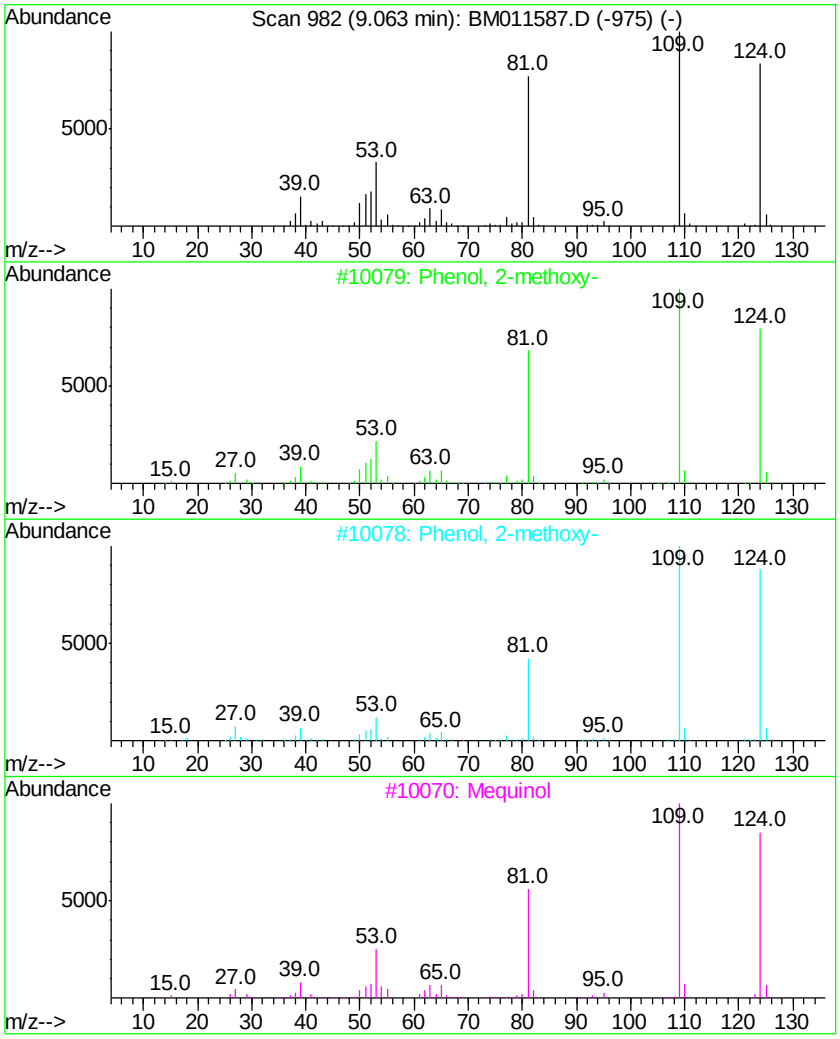
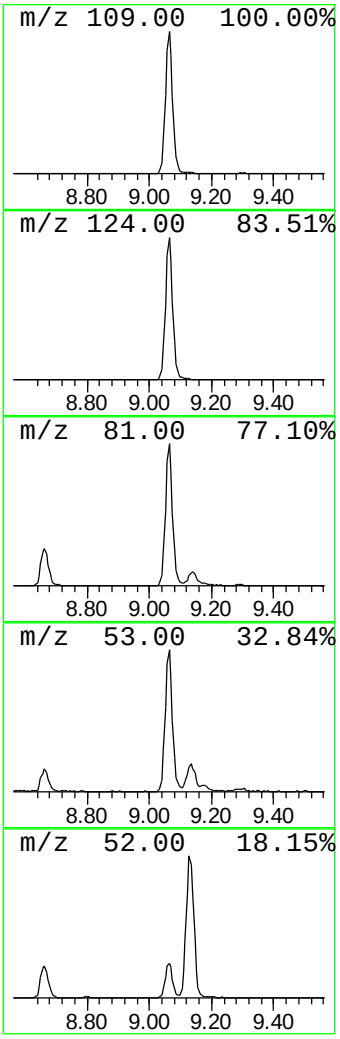
Peak Number 3 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	10.01 ng/ul	1456300	1,4-Dichlorobenzene-d4	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	93
3	Mequinol	124	C7H8O2	000150-76-5	93
4	Mequinol	124	C7H8O2	000150-76-5	90
5	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90





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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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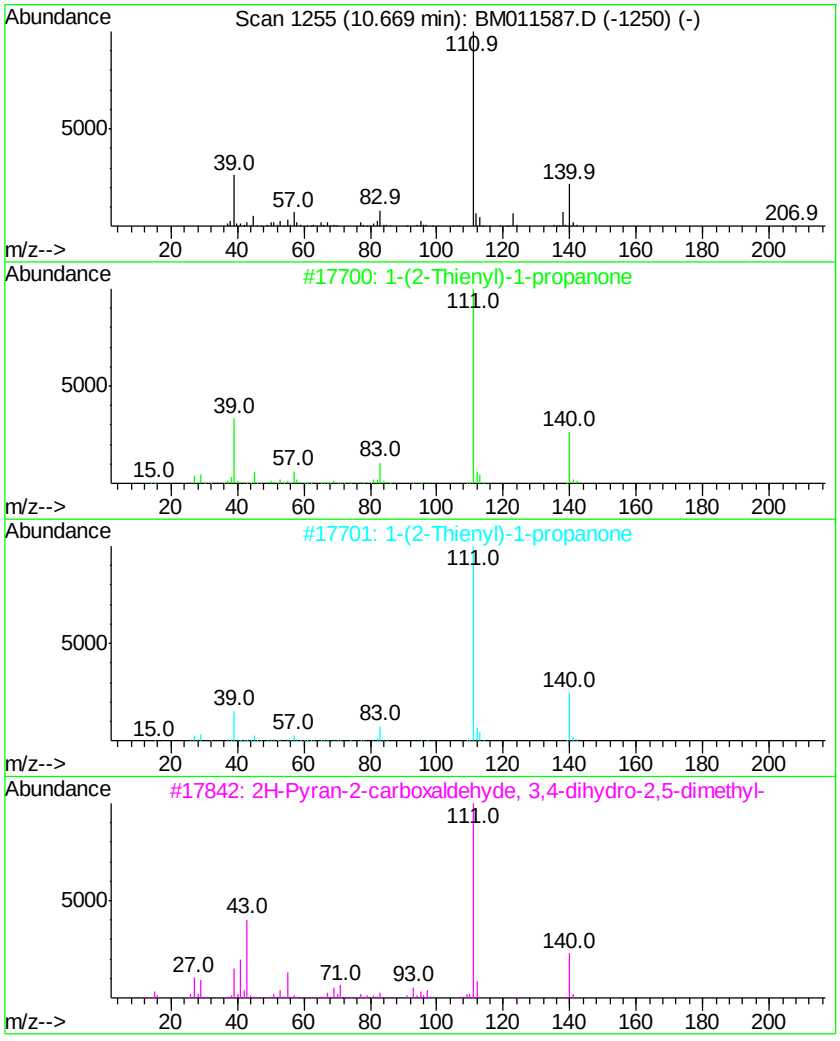
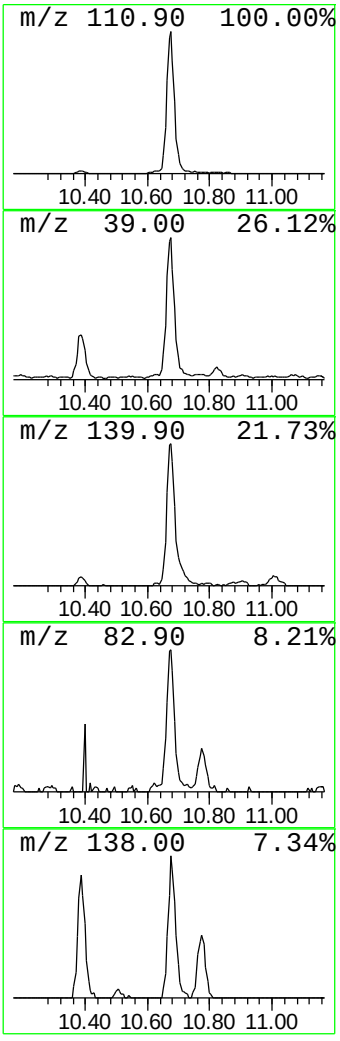
****

Peak Number 4 1-(2-Thienyl)-1-propanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.30 ng/ul	723214	Naphthalene-d8	10.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	81
2	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	72
3	2H-Pyran-2-carboxaldehyde, 3,4-d...	140	C8H12O2	001920-21-4	64
4	Thiophene-2-carboxylic acid, 2-a...	246	C13H10O3S	077708-28-2	50
5	p-Fluoroaniline	111	C6H6FN	000371-40-4	47





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Misc :
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Instrument : BNA_M
ClientSampleId : C0AC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

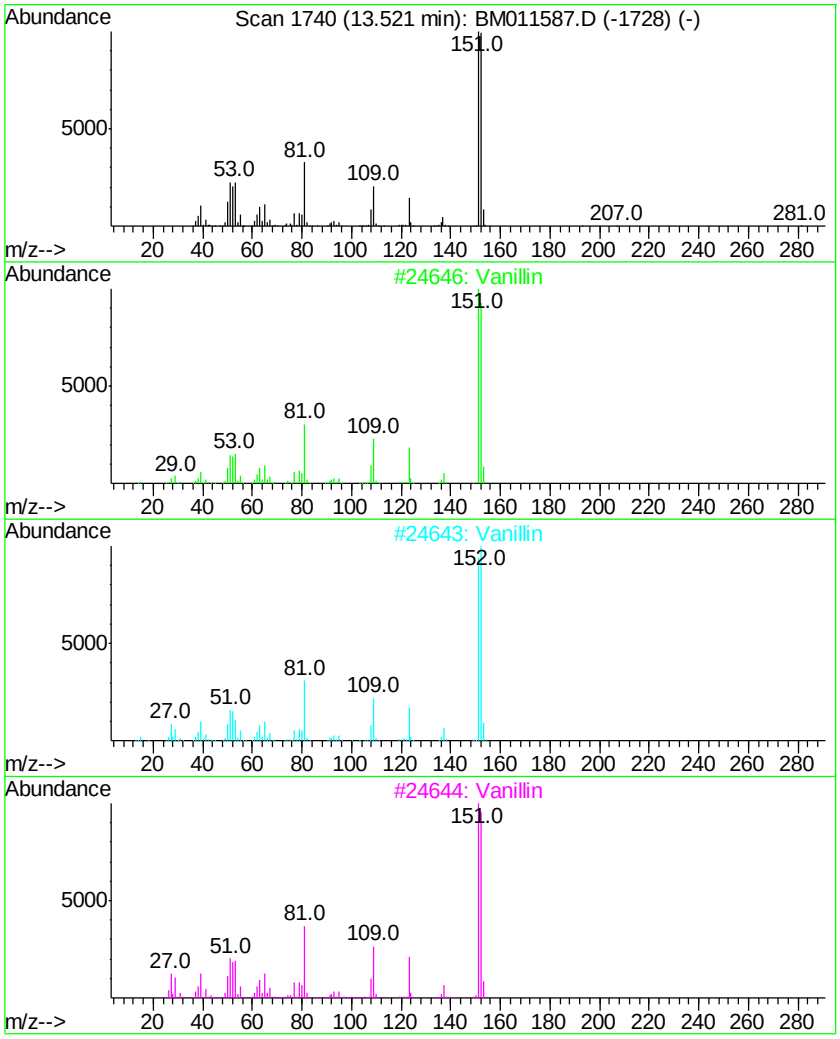
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

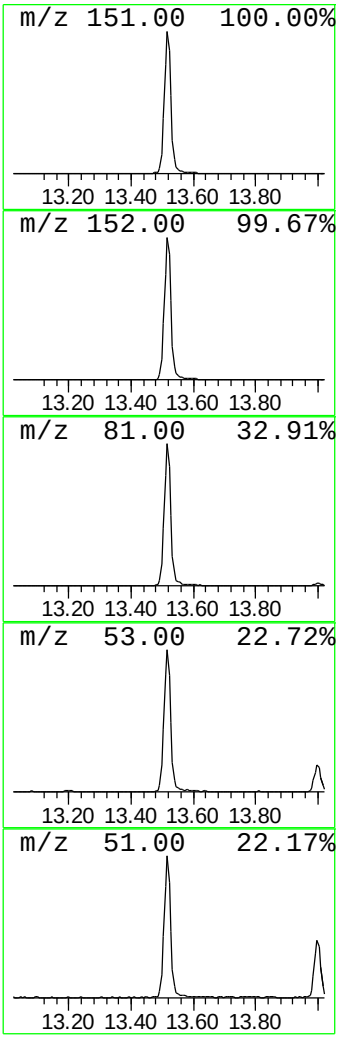
****

Peak Number 5 Vanillin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	12.48 ng/ul	3644680	Acenaphthene-d10	14.60

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	Vanillin	152	C8H8O3	000121-33-5	96
4	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
5	Vanillin	152	C8H8O3	000121-33-5	92





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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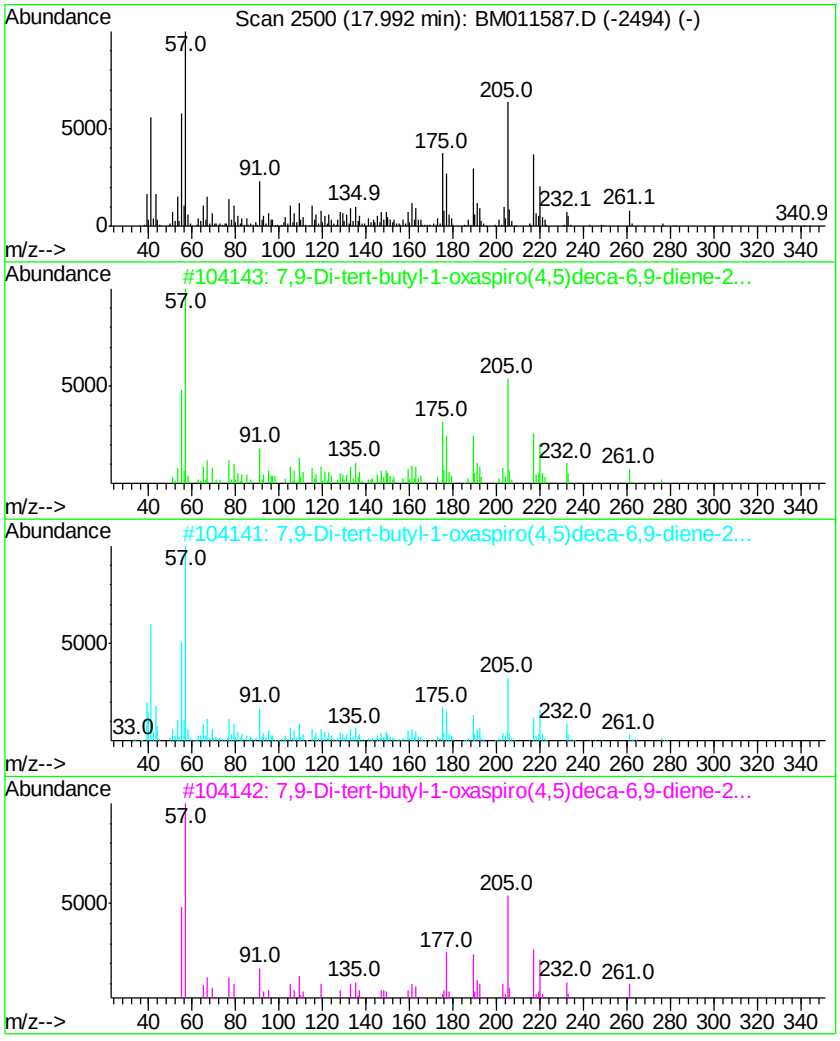
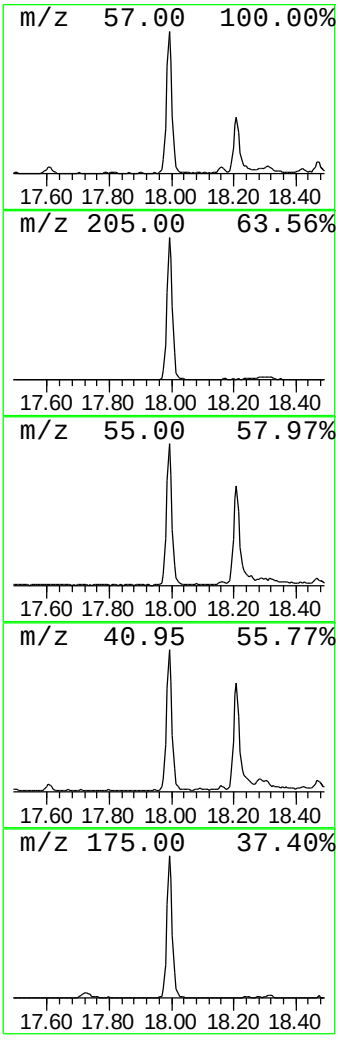
Peak Number 6 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	4.97 ng/ul	1696330	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	60
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	55
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	46
5	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	30





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM091817\
Data File : BM011587.D
Acq On : 19 Sep 2017 02:04
Operator : SJ/JU
Sample : I5271-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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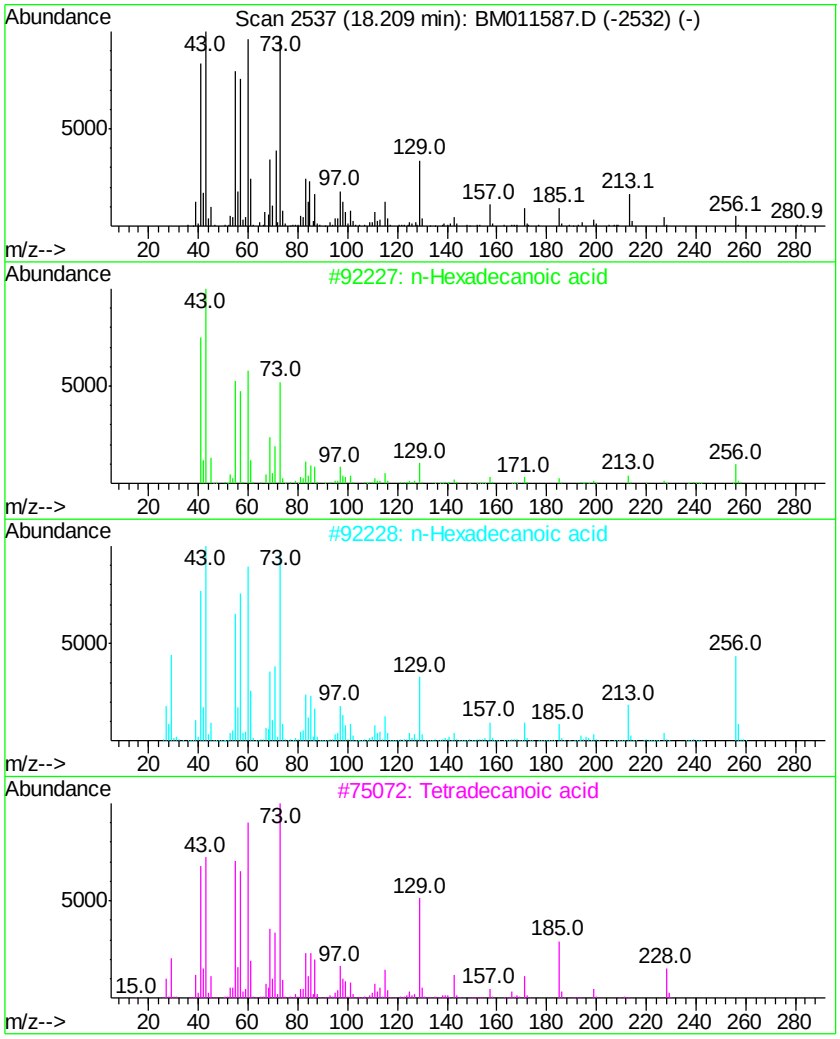
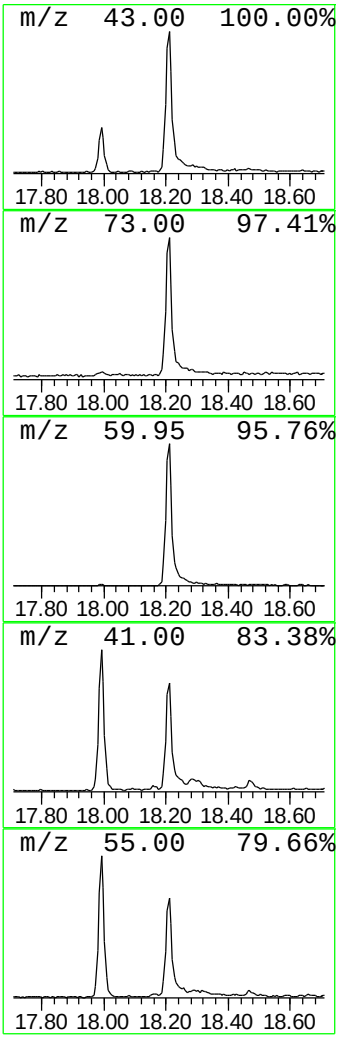
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	3.03 ng/ul	1032570	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM091817\
Data File : BM011587.D
Acq On : 19 Sep 2017 02:04
Operator : SJ/JU
Sample : I5271-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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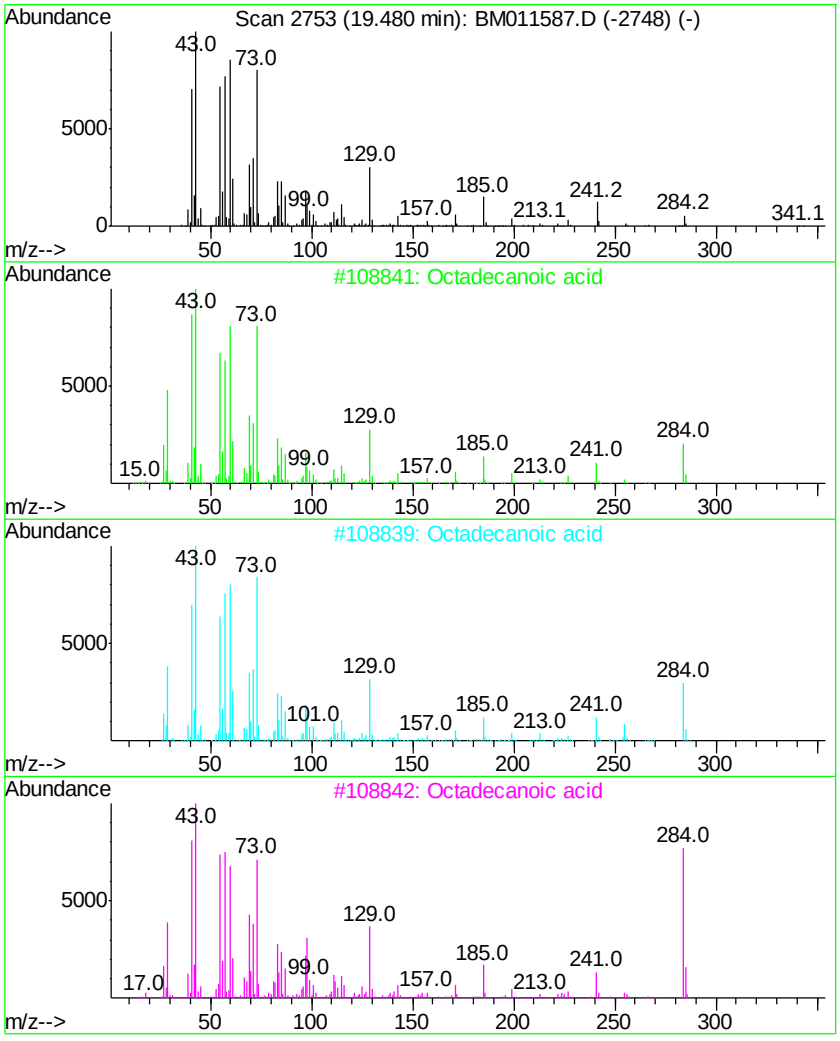
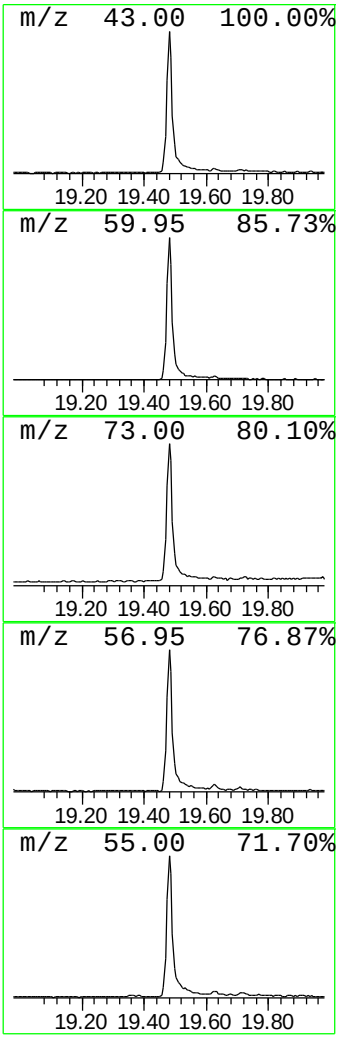
Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.48	6.34 ng/ul	2231060	Chrysene-d12	21.50

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	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	94
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091817\
Data File : BM011587.D
Acq On : 19 Sep 2017 02:04
Operator : SJ/JU
Sample : I5271-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC5

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexanone	6.01	35.4	ng/ul	5151150	1	7.97	2910490	20.0
1-Hexanol, 2-ethyl-	8.02	7.8	ng/ul	1141130	1	7.97	2910490	20.0
Phenol, 2-methoxy-	9.06	10.0	ng/ul	1456300	1	7.97	2910490	20.0
1-(2-Thienyl)-1-p...	10.67	3.3	ng/ul	723214	2	10.77	4381360	20.0
Vanillin	13.52	12.5	ng/ul	3644680	3	14.60	5840510	20.0
7,9-Di-tert-butyl...	17.99	5.0	ng/ul	1696330	4	17.34	6822920	20.0
n-Hexadecanoic acid	18.21	3.0	ng/ul	1032570	4	17.34	6822920	20.0
Octadecanoic acid	19.48	6.3	ng/ul	2231060	5	21.50	7036840	20.0