LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
Acq On : 19 Sep 2017 17:25
Operator : SJ/JU
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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	87775	129069	1.21%	0.113%
2	4.040	124	128	134	rVB4	13408	19123	0.18%	0.017%
3	4.146	142	146	150	rVB4	10701	17470	0.16%	0.015%
4	4.246	158	163	170	rBV4	14894	30200	0.28%	0.027%
5	4.504	203	207	211	rBV4	14078	22158	0.21%	0.019%
6	5.069	298	303	313	rVB	81716	143220	1.34%	0.126%
7	5.451	365	368	373	rBV4	15657	27109	0.25%	0.024%
8	5.499	373	376	381	rVB2	15953	22488	0.21%	0.020%
9	6.010	456	463	481	rBV	3157511	5005213	46.89%	4.399%
10	6.169	487	490	497	rVB5	9302	15462	0.14%	0.014%
11	6.616	562	566	572	rBV2	19003	31281	0.29%	0.027%
12	6.945	616	622	633	rBV5	29224	87790	0.82%	0.077%
13	7.057	636	641	645	rVV4	29232	61663	0.58%	0.054%
14	7.116	645	651	664	rVV	454480	829656	7.77%	0.729%
15	7.240	667	672	674	rBV3	11657	15573	0.15%	0.014%
16	7.293	674	681	693	rVV	1459752	2403938	22.52%	2.113%
17	7.492	708	715	730	rBV	1464812	2425067	22.72%	2.131%
18	7.751	753	759	762	rBV6	9524	18510	0.17%	0.016%
19	7.969	788	796	800	rBV	1326061	2191750	20.53%	1.926%
20	8.016	800	804	814	rVB	612820	1002186	9.39%	0.881%
21	8.222	834	839	841	rBV4	10321	16967	0.16%	0.015%
22	8.251	841	844	852	rVB5	16572	29284	0.27%	0.026%
23	8.581	894	900	905	rVV	45325	80121	0.75%	0.070%
24	8.663	907	914	927	rVV	1120700	1984283	18.59%	1.744%
25	8.792	931	936	944	rVB	53096	94656	0.89%	0.083%
26	9.063	975	982	987	rBV	806822	1367578	12.81%	1.202%
27	9.128	987	993	999	rVV	1836900	3149253	29.51%	2.768%
28	9.175	999	1001	1007	rVB	179423	246343	2.31%	0.217%
29	9.287	1014	1020	1029	rVB2	74531	166088	1.56%	0.146%
30	9.522	1055	1060	1067	rVB2	37187	62555	0.59%	0.055%
31	9.851	1108	1116	1134	rBV	1450378	2446925	22.93%	2.151%
32	9.998	1134	1141	1145	rBV10	12088	30147	0.28%	0.026%
33	10.186	1168	1173	1176	rBV6	6735	11284	0.11%	0.010%
34	10.275	1186	1188	1194	rVB6	10496	15674	0.15%	0.014%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
Acq On : 19 Sep 2017 17:25
Operator : SJ/JU
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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

35	10.386	1200	1207	1225	rBV	2024718	3493965	32.74%	3.071%
36	10.545	1229	1234	1238	rVV5	11147	14323	0.13%	0.013%
37	10.675	1249	1256	1265	rBV	362546	668298	6.26%	0.587%
38	10.775	1265	1273	1279	rVV	1984330	3419338	32.04%	3.005%
39	10.822	1279	1281	1290	rVV2	84828	121903	1.14%	0.107%
40	10.910	1291	1296	1304	rVV	56840	112334	1.05%	0.099%
41	11.004	1307	1312	1319	rVB3	16655	32324	0.30%	0.028%
42	11.304	1359	1363	1367	rBV4	9146	16704	0.16%	0.015%
43	11.369	1367	1374	1380	rBV3	8496	17673	0.17%	0.016%
44	11.433	1380	1385	1394	rVB5	22353	50553	0.47%	0.044%
45	11.545	1394	1404	1405	rBV6	16653	27982	0.26%	0.025%
46	11.763	1435	1441	1445	rBV6	14142	33970	0.32%	0.030%
47	11.933	1464	1470	1479	rBV3	48779	98241	0.92%	0.086%
48	12.039	1479	1488	1505	rVB2	519622	983110	9.21%	0.864%
49	12.357	1534	1542	1549	rVB3	44085	88786	0.83%	0.078%
50	12.663	1588	1594	1598	rBV4	10464	18200	0.17%	0.016%
51	12.804	1614	1618	1622	rBV6	8364	10980	0.10%	0.010%
52	12.863	1624	1628	1637	rBV4	35308	69089	0.65%	0.061%
53	12.951	1637	1643	1649	rVV2	56812	96531	0.90%	0.085%
54	13.057	1657	1661	1664	rBV3	10221	14402	0.13%	0.013%
55	13.198	1679	1685	1691	rBV	108344	160194	1.50%	0.141%
56	13.516	1728	1739	1762	rBV	2026389	3160730	29.61%	2.778%
57	13.998	1814	1821	1836	rVB	4112189	5738586	53.77%	5.044%
58	14.116	1836	1841	1846	rVB4	19260	26583	0.25%	0.023%
59	14.292	1864	1871	1884	rBV	4631104	6695325	62.73%	5.885%
60	14.457	1893	1899	1910	rVB2	48610	108665	1.02%	0.096%
61	14.598	1916	1923	1931	rBV2	2989051	4534400	42.48%	3.985%
62	14.669	1931	1935	1942	rVB	44334	69180	0.65%	0.061%
63	14.780	1949	1954	1964	rBV	198041	413206	3.87%	0.363%
64	15.004	1989	1992	1999	rVB8	8420	15866	0.15%	0.014%
65	15.180	2018	2022	2027	rVB3	13122	20193	0.19%	0.018%
66	15.263	2031	2036	2042	rBV	83385	126696	1.19%	0.111%
67	15.392	2048	2058	2067	rBV5	38653	91687	0.86%	0.081%
68	15.586	2084	2091	2102	rBV	6083919	8502339	79.66%	7.473%
69	15.698	2104	2110	2124	rVV	1880120	2671628	25.03%	2.348%
70	15.827	2127	2132	2137	rVV2	61263	93219	0.87%	0.082%
71	15.880	2137	2141	2143	rVB3	9794	13156	0.12%	0.012%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
Acq On : 19 Sep 2017 17:25
Operator : SJ/JU
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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

72	15.951	2147	2153	2161	rBV	47349	75667	0.71%	0.067%
73	16.157	2184	2188	2195	rBV6	7739	14557	0.14%	0.013%
74	16.921	2315	2318	2324	rVV5	11039	18113	0.17%	0.016%
75	16.998	2328	2331	2338	rVB2	19508	27316	0.26%	0.024%
76	17.127	2349	2353	2356	rBV4	8661	13046	0.12%	0.011%
77	17.339	2382	2389	2396	rBV2	3712772	5328156	49.92%	4.683%
78	17.433	2399	2405	2417	rVV	6655454	9465300	88.68%	8.319%
79	17.521	2417	2420	2424	rVB5	21624	26406	0.25%	0.023%
80	17.604	2429	2434	2440	rVB	41069	57968	0.54%	0.051%
81	17.992	2495	2500	2511	rVB	1028734	1296174	12.14%	1.139%
82	18.162	2524	2529	2532	rBV4	18695	26873	0.25%	0.024%
83	18.204	2532	2536	2543	rVV3	68708	107226	1.00%	0.094%
84	18.286	2546	2550	2558	rVB2	51140	105795	0.99%	0.093%
85	18.421	2570	2573	2576	rBV4	16449	18631	0.17%	0.016%
86	18.474	2578	2582	2586	rBV	36142	46267	0.43%	0.041%
87	19.356	2726	2732	2739	rBV	62075	106908	1.00%	0.094%
88	19.474	2748	2752	2763	rBV3	95479	167264	1.57%	0.147%
89	19.609	2771	2775	2781	rVB2	49633	87600	0.82%	0.077%
90	19.721	2788	2794	2804	rBV	8374503	10673364	100.00%	9.381%
91	20.662	2952	2954	2959	rBV6	22525	29466	0.28%	0.026%
92	21.503	3091	3097	3105	rBV	4537961	5753030	53.90%	5.056%
93	22.574	3275	3279	3287	rBV	264331	392896	3.68%	0.345%
94	23.721	3467	3474	3485	rBV2	4730136	8998369	84.31%	7.909%
95	23.874	3493	3500	3514	rVB	2466822	4910590	46.01%	4.316%

Sum of corrected areas: 113777425

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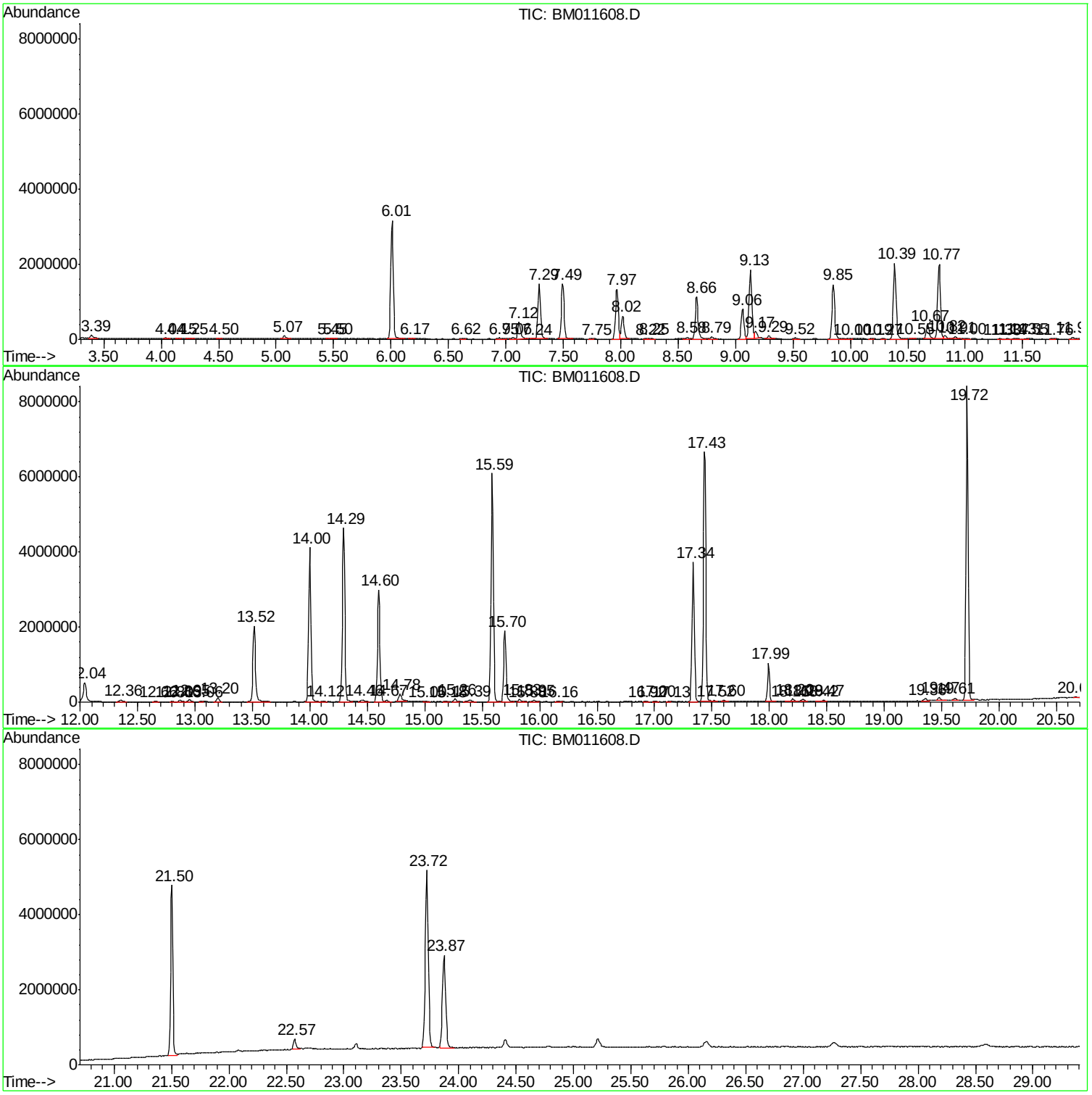
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM090817MA.M
Quant Title : SVOA CALIBRATION

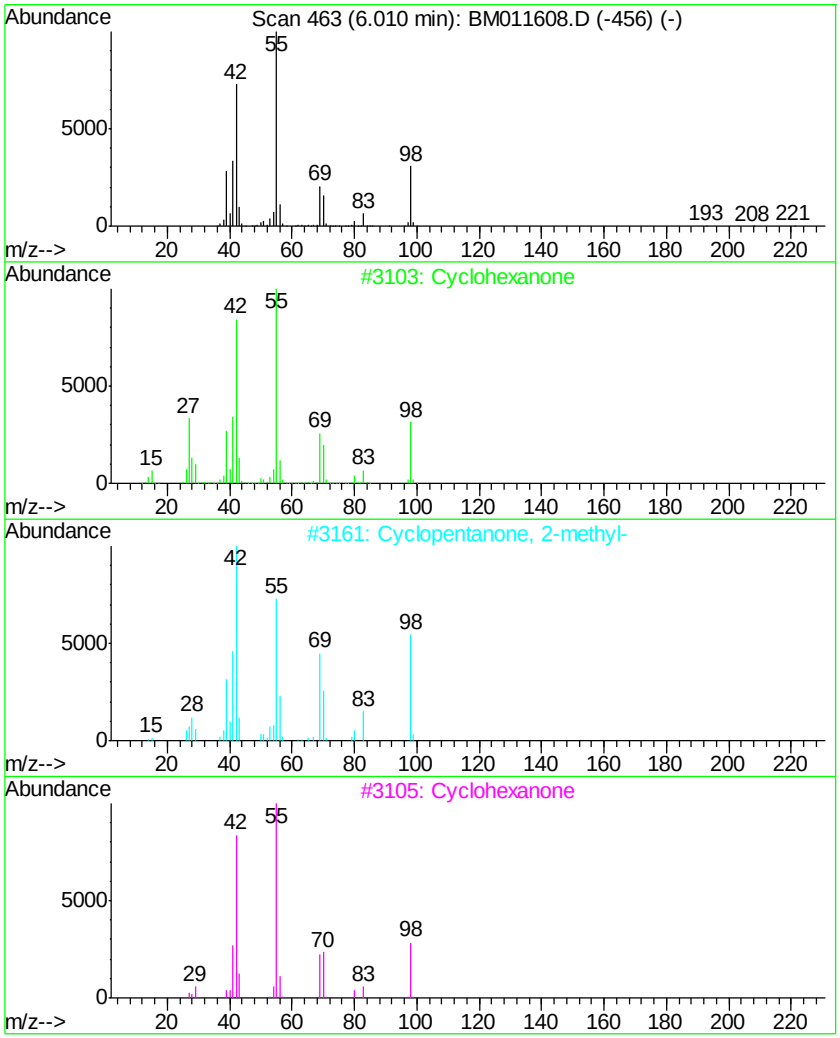
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

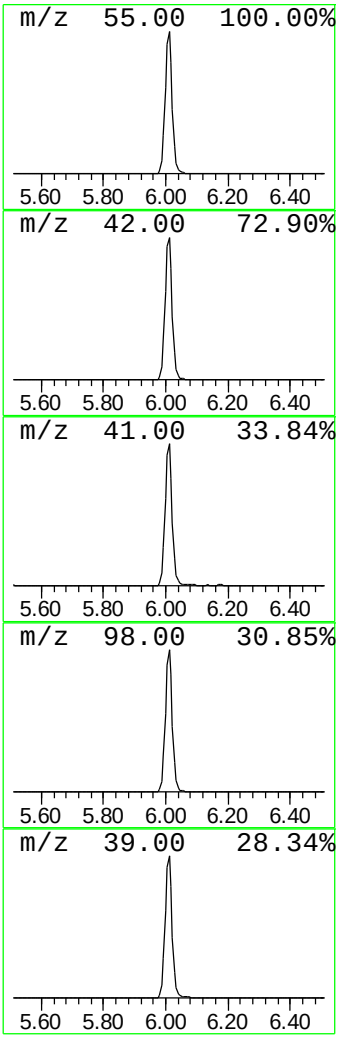
****

Peak Number 1 Cyclohexanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.01	45.67 ng/ul	5005210	1,4-Dichlorobenzene-d4	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	94
2	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	83
3	Cyclohexanone	98	C6H10O	000108-94-1	80
4	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	80
5	Cyclohexanone	98	C6H10O	000108-94-1	76





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
Acq On : 19 Sep 2017 17:25
Operator : SJ/JU
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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

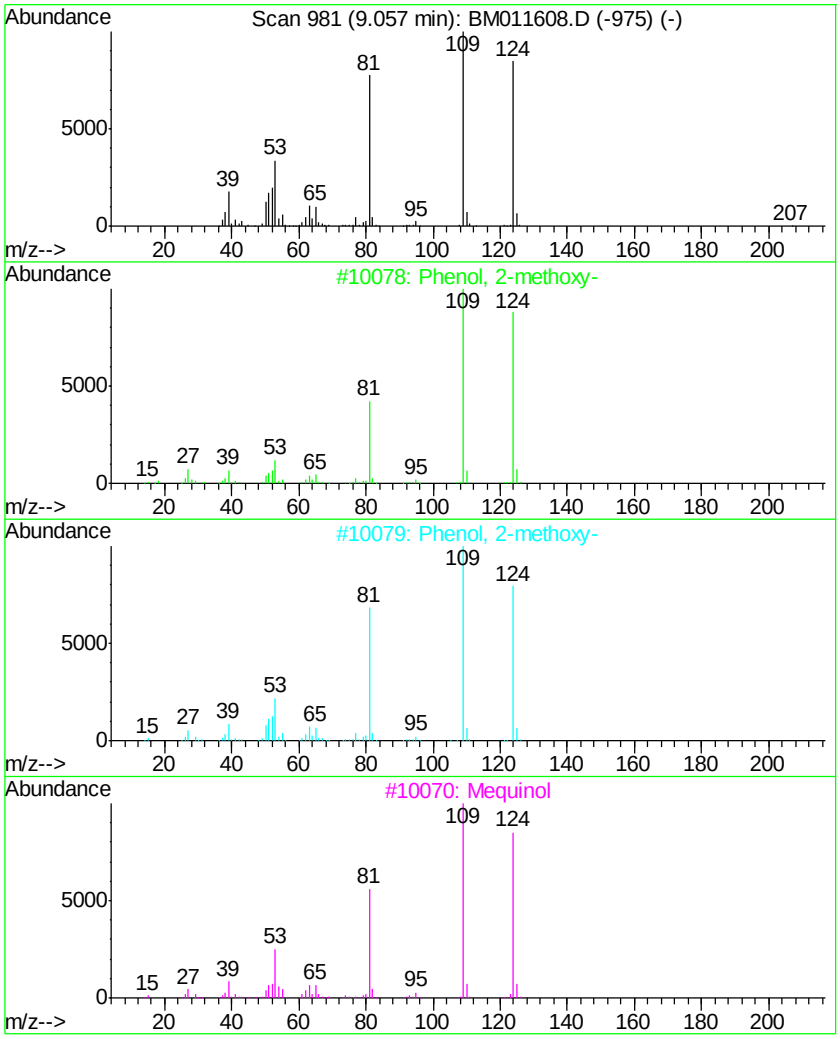
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

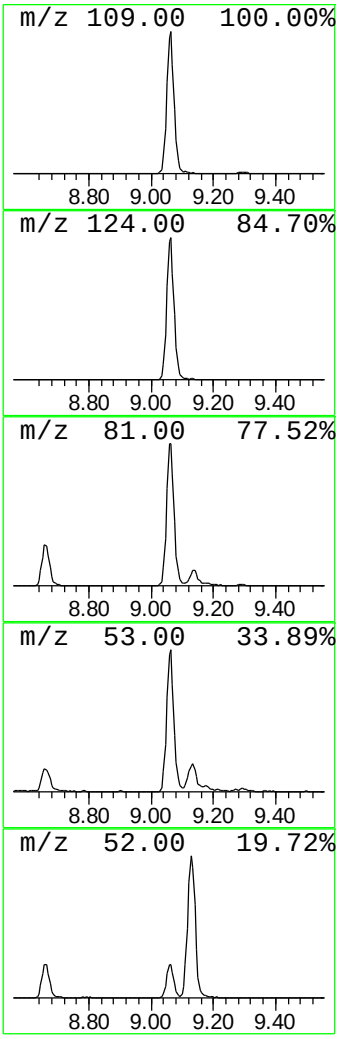
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	12.48 ng/ul	1367580	1,4-Dichlorobenzene-d4	7.97

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	93
4	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
5	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	70





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Sample : I5271-10
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Instrument : BNA_M
ClientSampleId : C0AE2

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

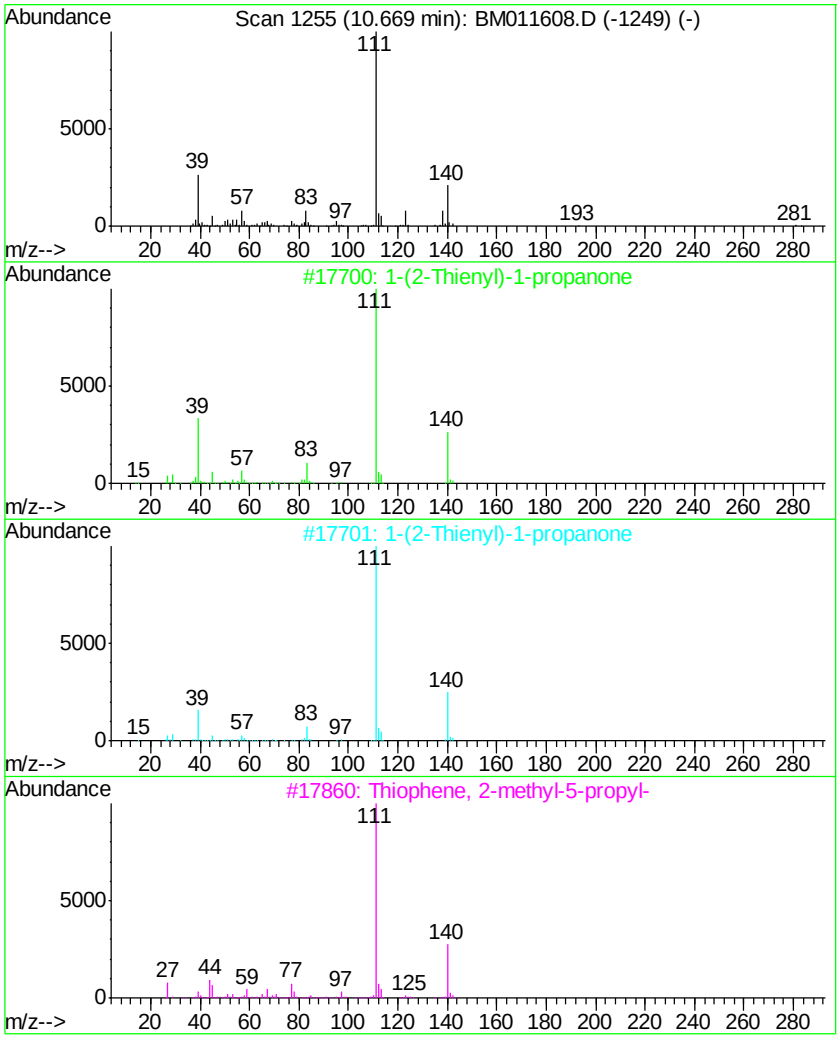
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

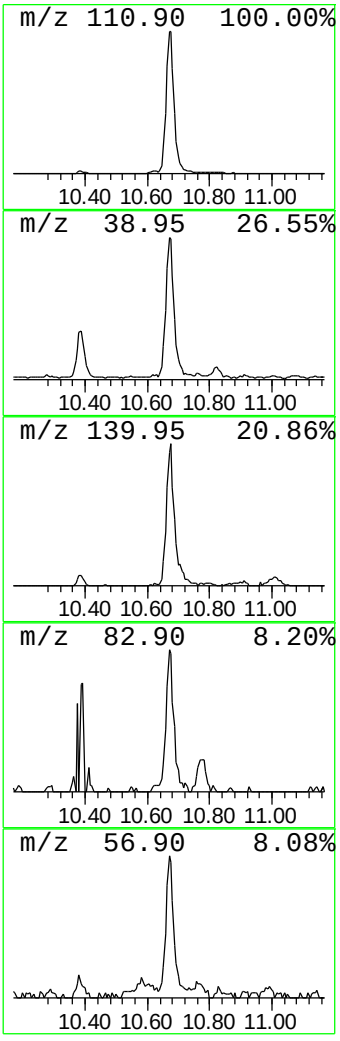
****

Peak Number 3 1-(2-Thienyl)-1-propanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.91 ng/ul	668298	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	Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	64
4	Butane-1,4-dione, 1,4-bis(2-thie...	250	C12H10O2S2	013669-05-1	50
5	p-Fluoroaniline	111	C6H6FN	000371-40-4	49





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
Acq On : 19 Sep 2017 17:25
Operator : SJ/JU
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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

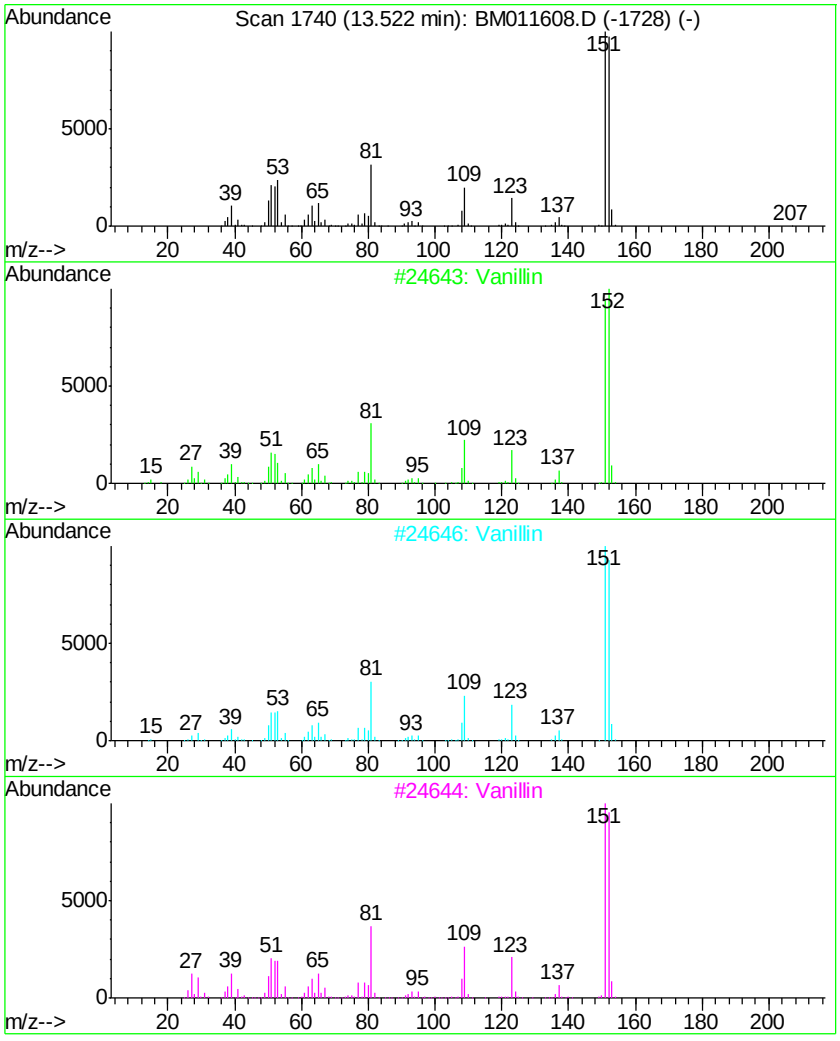
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

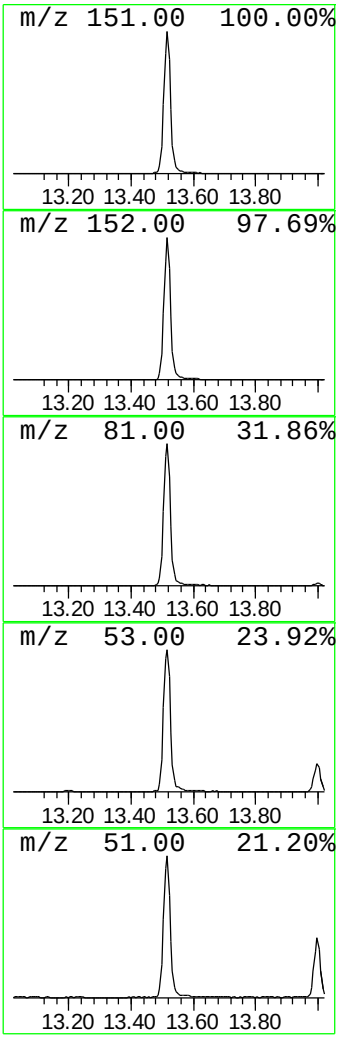
****

Peak Number 4 Vanillin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	13.94 ng/ul	3160730	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	96
3	Vanillin	152	C8H8O3	000121-33-5	96
4	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
Acq On : 19 Sep 2017 17:25
Operator : SJ/JU
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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

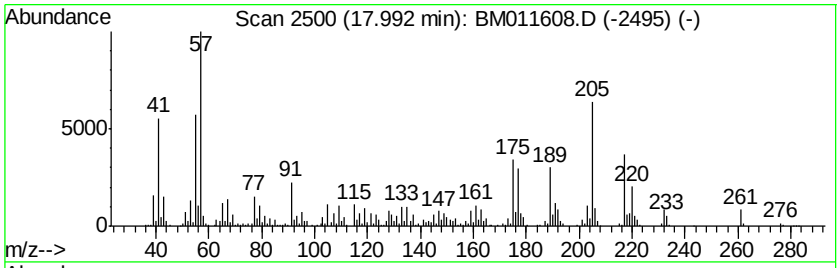
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

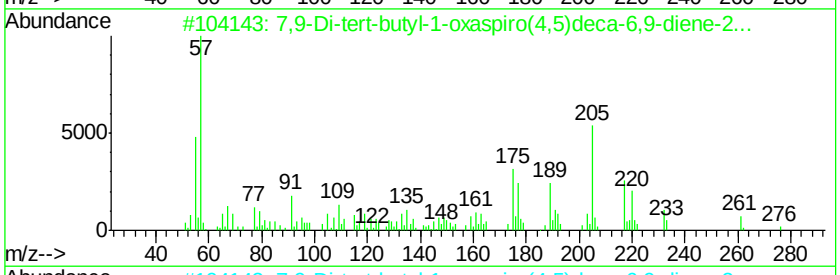
****

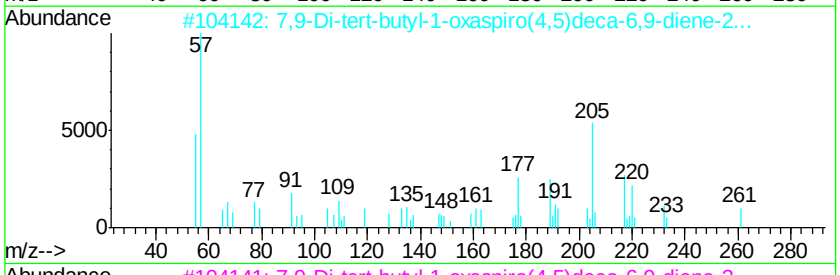
Peak Number 5 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 4

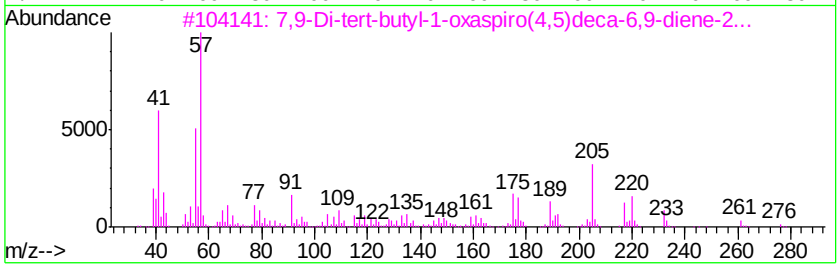
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	4.87 ng/ul	1296170	Phenanthrene-d10	17.34

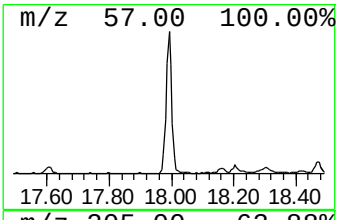
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	87
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	64
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	46
5	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	38

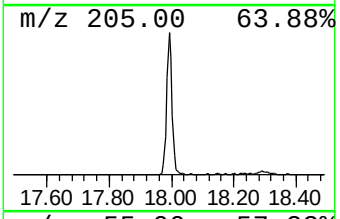


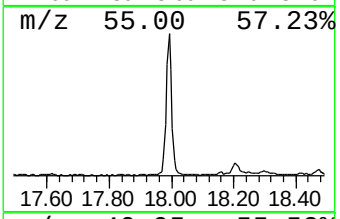


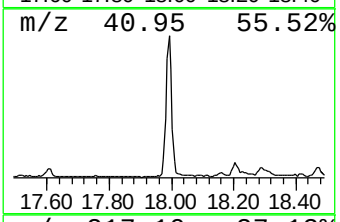


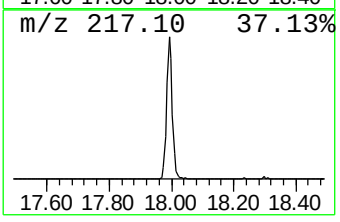












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM091917\
Data File : BM011608.D
Acq On : 19 Sep 2017 17:25
Operator : SJ/JU
Sample : I5271-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AE2

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	45.7	ng/ul	5005210	1	7.97	2191750	20.0
Phenol, 2-methoxy-	9.06	12.5	ng/ul	1367580	1	7.97	2191750	20.0
1-(2-Thienyl)-1-p...	10.67	3.9	ng/ul	668298	2	10.77	3419340	20.0
Vanillin	13.52	13.9	ng/ul	3160730	3	14.60	4534400	20.0
7,9-Di-tert-butyl...	17.99	4.9	ng/ul	1296170	4	17.34	5328160	20.0