LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM092017\
Data File : BM011638.D
Acq On : 20 Sep 2017 15:32
Operator : SJ/JU
Sample : I5273-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC6

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	3.387	14	17	27	rBV	76609	114391	1.16%	0.101%
2	4.504	201	207	213	rVB6	14556	26902	0.27%	0.024%
3	5.069	298	303	312	rBV	74063	118529	1.20%	0.105%
4	5.275	332	338	347	rBV	196703	327869	3.32%	0.289%
5	6.004	455	462	479	rBV	2552396	3978431	40.29%	3.511%
6	6.939	614	621	630	rBV2	24020	66644	0.67%	0.059%
7	7.057	636	641	645	rBV4	19409	33984	0.34%	0.030%
8	7.110	645	650	662	rVB	309479	590571	5.98%	0.521%
9	7.287	674	680	694	rVV	1279553	2009825	20.35%	1.774%
10	7.492	708	715	730	rBV	1235097	2037258	20.63%	1.798%
11	7.857	770	777	782	rVB3	18730	35563	0.36%	0.031%
12	7.963	787	795	800	rBV	1392275	2323667	23.53%	2.051%
13	8.016	800	804	816	rVB2	443436	809877	8.20%	0.715%
14	8.316	850	855	864	rVB	127351	225575	2.28%	0.199%
15	8.581	894	900	906	rVV	32765	61099	0.62%	0.054%
16	8.657	906	913	931	rVV	902203	1579652	16.00%	1.394%
17	8.792	931	936	942	rVB2	40210	69725	0.71%	0.062%
18	9.057	973	981	987	rBV	595071	1017840	10.31%	0.898%
19	9.128	987	993	998	rVV	1606202	2686232	27.20%	2.371%
20	9.169	998	1000	1006	rVB	118734	190558	1.93%	0.168%
21	9.281	1014	1019	1033	rVB2	113623	249684	2.53%	0.220%
22	9.516	1055	1059	1066	rVB3	22604	37534	0.38%	0.033%
23	9.845	1105	1115	1126	rBV	1282092	2267793	22.97%	2.001%
24	9.928	1127	1129	1135	rVB6	13623	24402	0.25%	0.022%
25	10.080	1149	1155	1160	rVB7	14888	30926	0.31%	0.027%
26	10.198	1166	1175	1179	rBV8	14039	44185	0.45%	0.039%
27	10.380	1199	1206	1222	rBV	1772264	3069744	31.09%	2.709%
28	10.627	1243	1248	1250	rVV3	75144	115679	1.17%	0.102%
29	10.669	1250	1255	1262	rVV	258378	535416	5.42%	0.472%
30	10.769	1265	1272	1278	rVV	2056316	3549627	35.95%	3.133%
31	10.816	1278	1280	1287	rVV3	76881	126572	1.28%	0.112%
32	10.910	1291	1296	1302	rVV3	57392	115956	1.17%	0.102%
33	11.004	1305	1312	1317	rVB6	16457	42538	0.43%	0.038%
34	11.151	1332	1337	1342	rVB8	12770	31180	0.32%	0.028%

LSC Area Percent Report

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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

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	11.433	1378	1385	1386	rBV2	35042	62294	0.63%	0.055%
36	11.457	1386	1389	1396	rVB2	45177	79329	0.80%	0.070%
37	11.539	1396	1403	1408	rBV7	30299	76297	0.77%	0.067%
38	11.686	1421	1428	1434	rBV9	14819	33467	0.34%	0.030%
39	11.774	1434	1443	1447	rBV	90887	181723	1.84%	0.160%
40	11.810	1447	1449	1454	rVV5	23104	31771	0.32%	0.028%
41	11.863	1456	1458	1464	rVB5	17068	25053	0.25%	0.022%
42	11.927	1464	1469	1479	rBV2	44970	97491	0.99%	0.086%
43	12.039	1479	1488	1502	rBV	372285	764001	7.74%	0.674%
44	12.163	1505	1509	1514	rBV5	17287	27270	0.28%	0.024%
45	12.257	1520	1525	1531	rBV7	21562	43637	0.44%	0.039%
46	12.357	1537	1542	1552	rVB6	52469	154149	1.56%	0.136%
47	12.651	1589	1592	1601	rVB5	21603	44360	0.45%	0.039%
48	12.792	1611	1616	1623	rVB4	60571	105790	1.07%	0.093%
49	12.863	1623	1628	1637	rBV2	75990	140056	1.42%	0.124%
50	12.945	1637	1642	1647	rBV	50984	89807	0.91%	0.079%
51	13.051	1656	1660	1664	rBV4	13132	24605	0.25%	0.022%
52	13.116	1667	1671	1677	rVV	94273	139519	1.41%	0.123%
53	13.192	1677	1684	1690	rVB	94003	144366	1.46%	0.127%
54	13.398	1714	1719	1720	rBV4	21055	27900	0.28%	0.025%
55	13.433	1722	1725	1729	rVV3	24038	36740	0.37%	0.032%
56	13.510	1729	1738	1754	rVV	1498210	2499743	25.32%	2.206%
57	13.998	1814	1821	1827	rVV	3638583	5239510	53.06%	4.624%
58	14.063	1827	1832	1836	rVB3	159117	264754	2.68%	0.234%
59	14.110	1836	1840	1846	rVB5	38751	58818	0.60%	0.052%
60	14.233	1857	1861	1864	rBV4	18980	28401	0.29%	0.025%
61	14.292	1864	1871	1882	rBV	4044612	6076228	61.53%	5.362%
62	14.457	1894	1899	1903	rVV2	35709	58217	0.59%	0.051%
63	14.551	1910	1915	1916	rBV2	31206	40970	0.41%	0.036%
64	14.592	1916	1922	1932	rVV2	3100540	4881111	49.43%	4.308%
65	14.674	1932	1936	1939	rVB5	36638	52790	0.53%	0.047%
66	14.780	1950	1954	1966	rVV4	123724	276012	2.80%	0.244%
67	14.980	1984	1988	1994	rBV4	36352	58754	0.60%	0.052%
68	15.092	2003	2007	2014	rVB5	28002	50792	0.51%	0.045%
69	15.257	2031	2035	2040	rBV	82589	129189	1.31%	0.114%
70	15.321	2040	2046	2052	rVB3	33957	68119	0.69%	0.060%
71	15.398	2052	2059	2064	rBV6	59698	135151	1.37%	0.119%

LSC Area Percent Report

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

72	15.527	2078	2081	2084	rBV3	20307	26598	0.27%	0.023%
73	15.586	2084	2091	2098	rBV	5258255	7696161	77.94%	6.792%
74	15.692	2103	2109	2123	rVV	1745111	2551663	25.84%	2.252%
75	15.827	2126	2132	2137	rVB	233486	368688	3.73%	0.325%
76	15.945	2148	2152	2157	rVB	47389	74392	0.75%	0.066%
77	16.304	2205	2213	2218	rBV	311915	474761	4.81%	0.419%
78	16.415	2226	2232	2233	rBV6	16823	28709	0.29%	0.025%
79	16.686	2275	2278	2281	rVB4	27586	31845	0.32%	0.028%
80	16.998	2328	2331	2337	rVB6	26310	40116	0.41%	0.035%
81	17.127	2347	2353	2364	rVB	189194	322309	3.26%	0.284%
82	17.333	2382	2388	2397	rBV2	4095615	5865608	59.40%	5.176%
83	17.433	2399	2405	2415	rVB2	6088831	8514246	86.22%	7.514%
84	17.604	2430	2434	2443	rVB	46876	78551	0.80%	0.069%
85	17.733	2451	2456	2461	rVB3	53143	83898	0.85%	0.074%
86	17.992	2494	2500	2508	rVB	904983	1209010	12.24%	1.067%
87	18.203	2531	2536	2546	rBV	338218	498390	5.05%	0.440%
88	18.286	2546	2550	2558	rVB2	71766	149019	1.51%	0.132%
89	18.468	2577	2581	2586	rVB2	44718	67983	0.69%	0.060%
90	19.350	2726	2731	2739	rBV2	67916	128157	1.30%	0.113%
91	19.474	2747	2752	2763	rBV	694353	1048213	10.62%	0.925%
92	19.609	2771	2775	2784	rVB2	57534	116426	1.18%	0.103%
93	19.721	2787	2794	2806	rBV	6982686	9874466	100.00%	8.714%
94	21.497	3091	3096	3105	rBV	5232325	6582195	66.66%	5.809%
95	22.568	3274	3278	3283	rBV	254738	368155	3.73%	0.325%
96	23.103	3366	3369	3375	rVB2	176064	258869	2.62%	0.228%
97	23.721	3466	3474	3489	rVB2	4553376	9136265	92.52%	8.063%
98	23.868	3492	3499	3512	rVB	2832104	5796325	58.70%	5.115%
99	24.403	3586	3590	3600	rVB	260915	513626	5.20%	0.453%
100	25.209	3722	3727	3738	rVB	268421	617838	6.26%	0.545%

Sum of corrected areas: 113316094

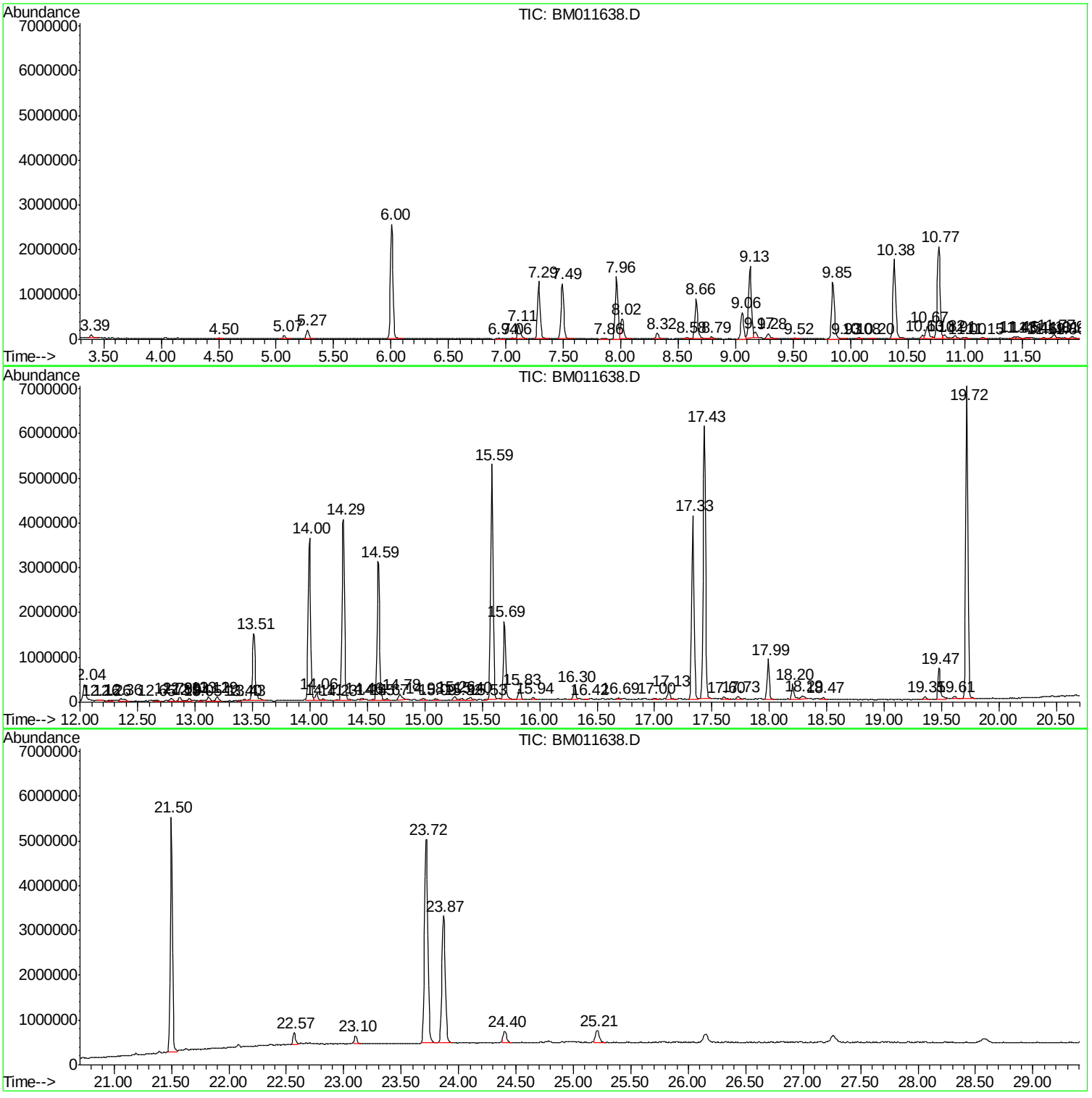
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM092017\
Data File : BM011638.D
Acq On : 20 Sep 2017 15:32
Operator : SJ/JU
Sample : I5273-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC6

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

Data Path : Z:\HPCHEM1\BNA M\DATA\BM092017\
Data File : BM011638.D
Acq On : 20 Sep 2017 15:32
Operator : SJ/JU
Sample : I5273-11
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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

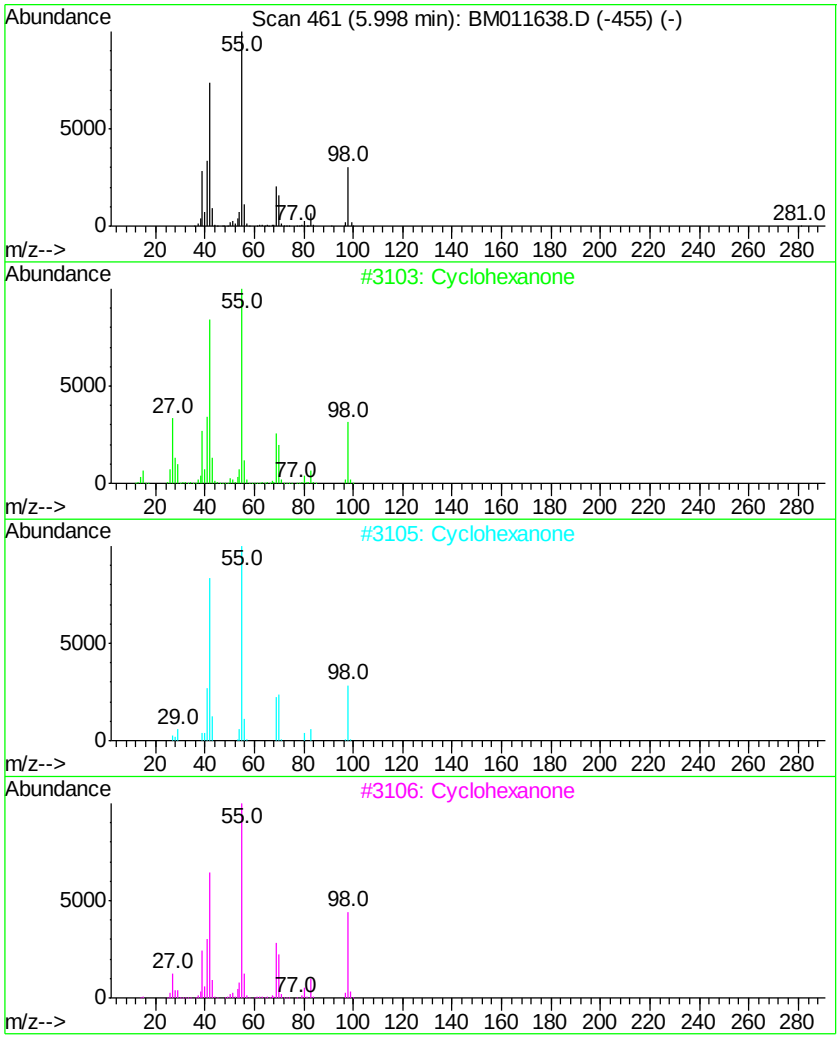
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

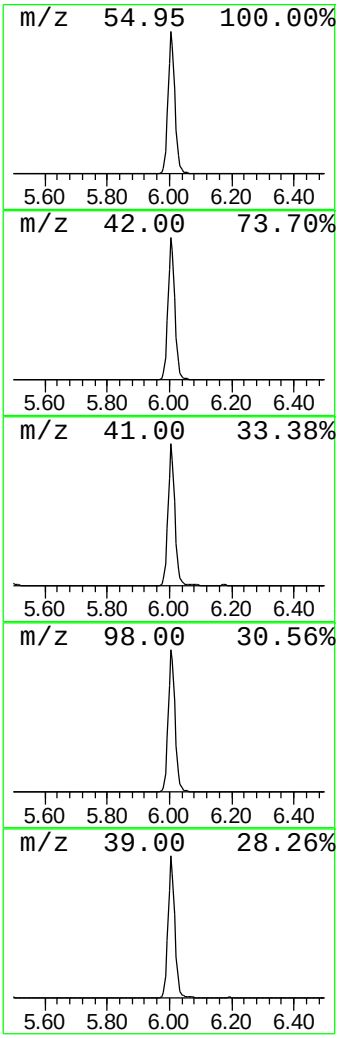
****

Peak Number 2 Cyclohexanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.00	34.24 ng/ul	3978430	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	94
2	Cyclohexanone	98	C6H10O	000108-94-1	80
3	Cyclohexanone	98	C6H10O	000108-94-1	64
4	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	53
5	2-Pentene	70	C5H10	000109-68-2	53





Data Path : Z:\HPCHEM1\BNA M\DATA\BM092017\
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Operator : SJ/JU
Sample : I5273-11
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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

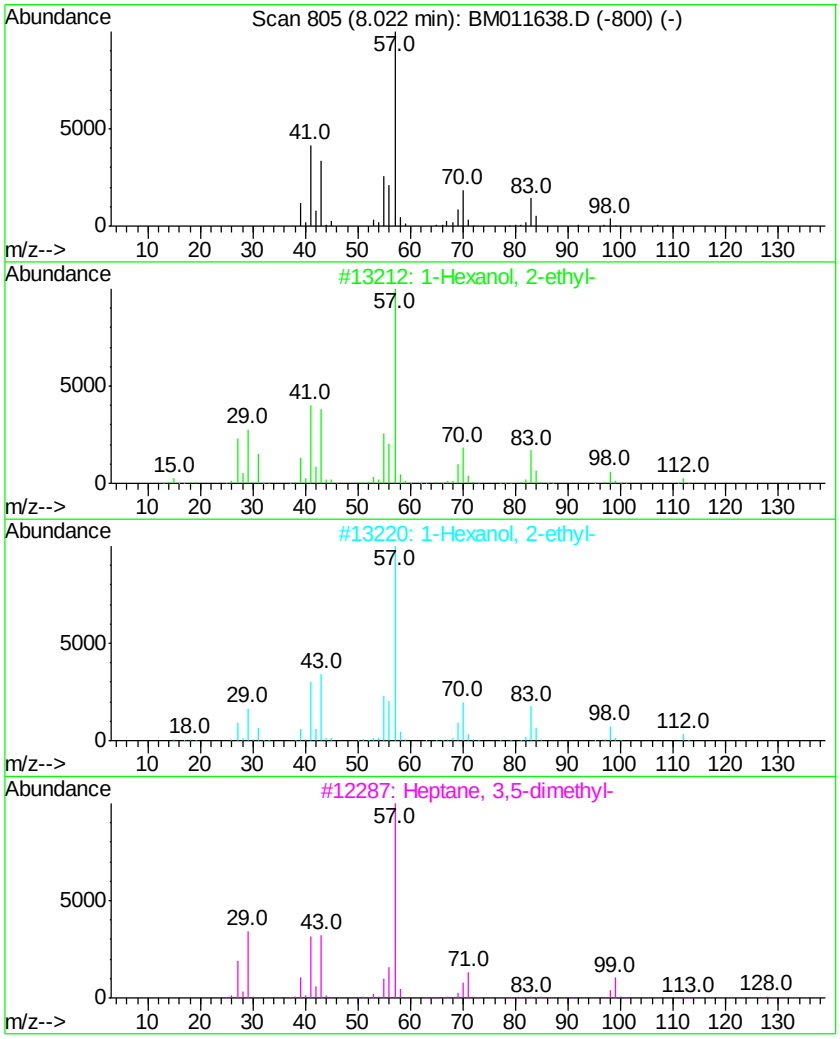
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

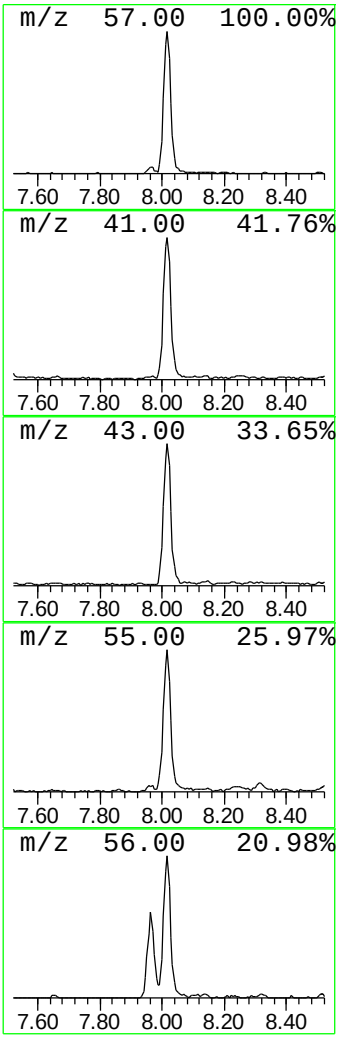
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.02	6.97 ng/ul	809877	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	45
4	4-Bromoheptane	178	C7H15Br	000998-93-6	43
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	42





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Quant Title : SVOA CALIBRATION

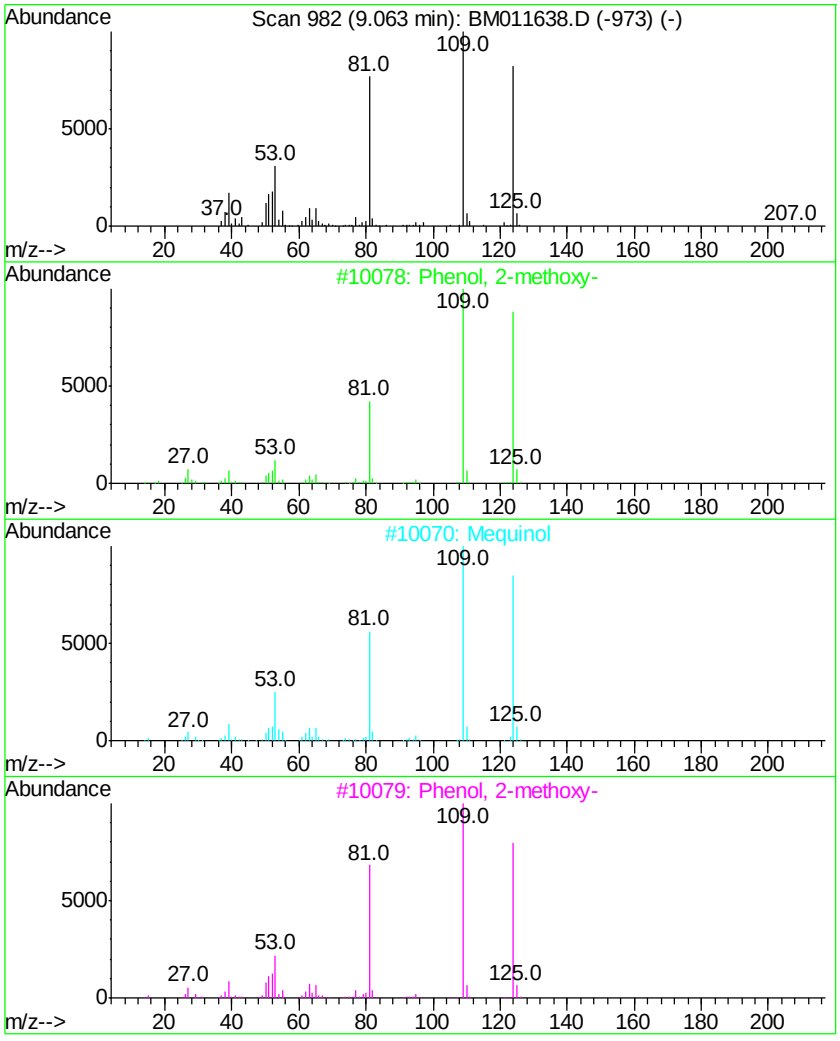
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

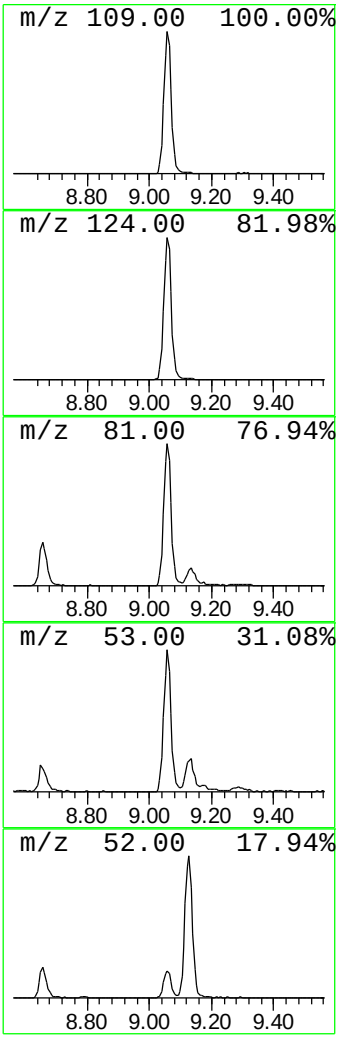
****

Peak Number 4 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	8.76 ng/ul	1017840	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	97
2	Mequinol	124	C7H8O2	000150-76-5	95
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
4	Mequinol	124	C7H8O2	000150-76-5	93
5	Mequinol	124	C7H8O2	000150-76-5	91





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

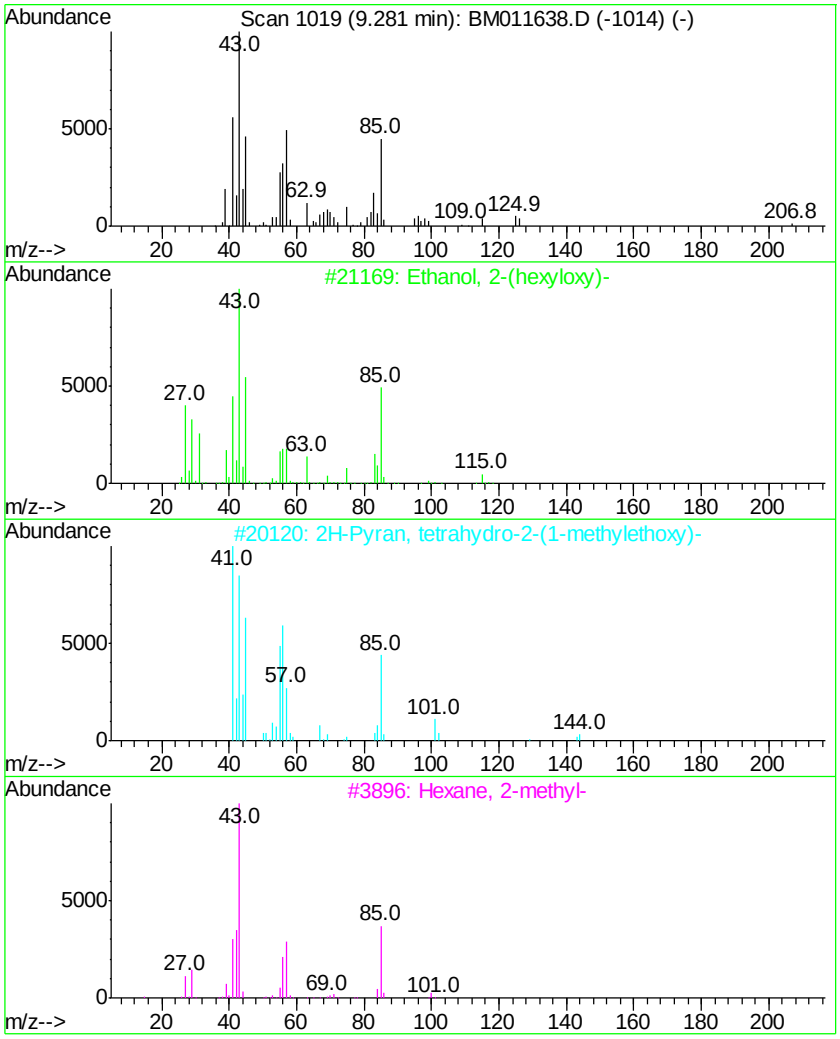
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

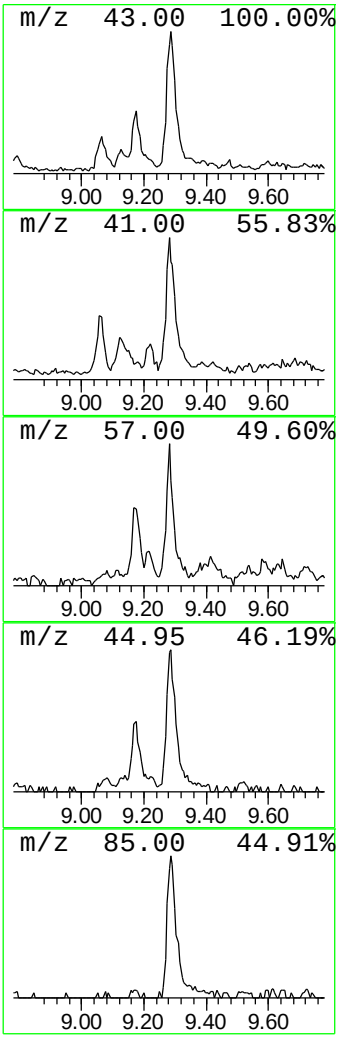
****

Peak Number 5 Ethanol, 2-(hexyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.28	2.15 ng/ul	249684	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexyloxy)-	146	C8H18O2	000112-25-4	59
2	2H-Pyran, tetrahydro-2-(1-methyl...	144	C8H16O2	001927-70-4	47
3	Hexane, 2-methyl-	100	C7H16	000591-76-4	35
4	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	32
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	25





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC6

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

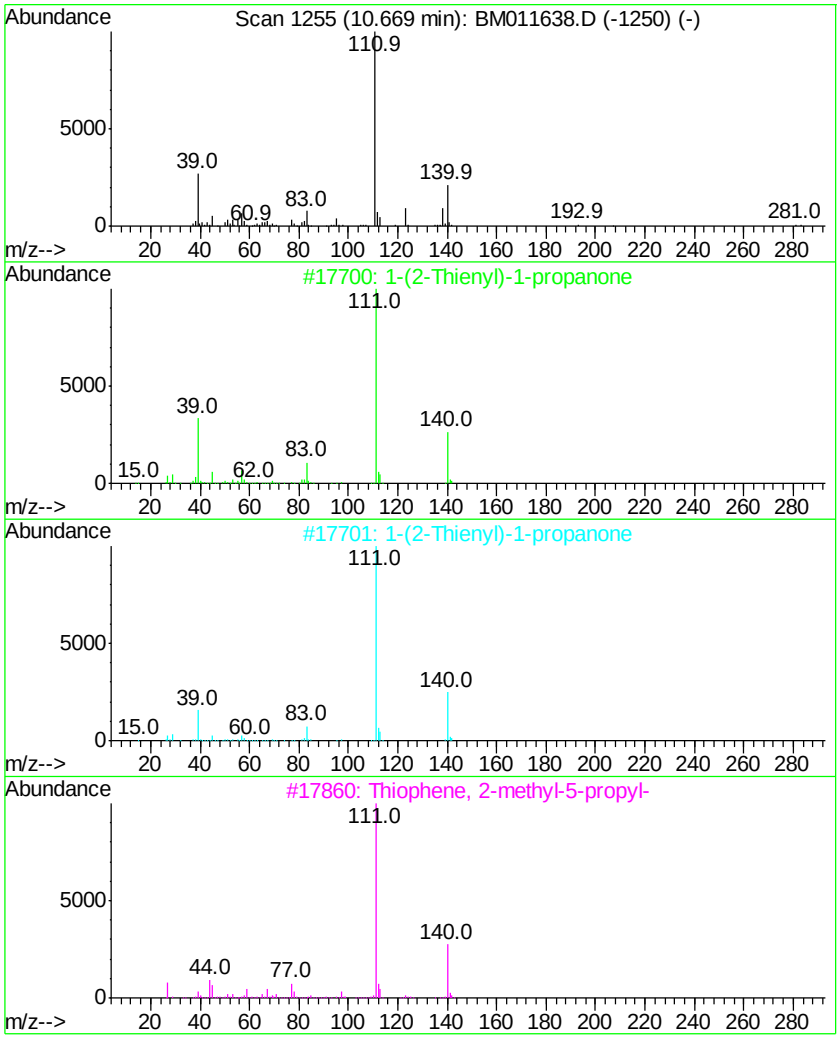
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

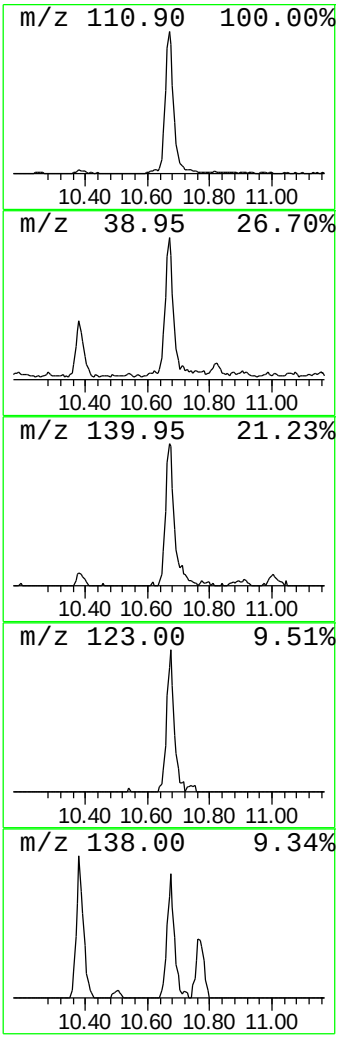
****

Peak Number 6 1-(2-Thienyl)-1-propanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.02 ng/ul	535416	Naphthalene-d8	10.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	76
2	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	64
3	Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	64
4	2H-Pyran-2-carboxaldehyde, 3,4-d...	140	C8H12O2	001920-21-4	59
5	1-Butanone, 1-(2-thienyl)-	154	C8H10OS	005333-83-5	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM092017\
Data File : BM011638.D
Acq On : 20 Sep 2017 15:32
Operator : SJ/JU
Sample : I5273-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AC6

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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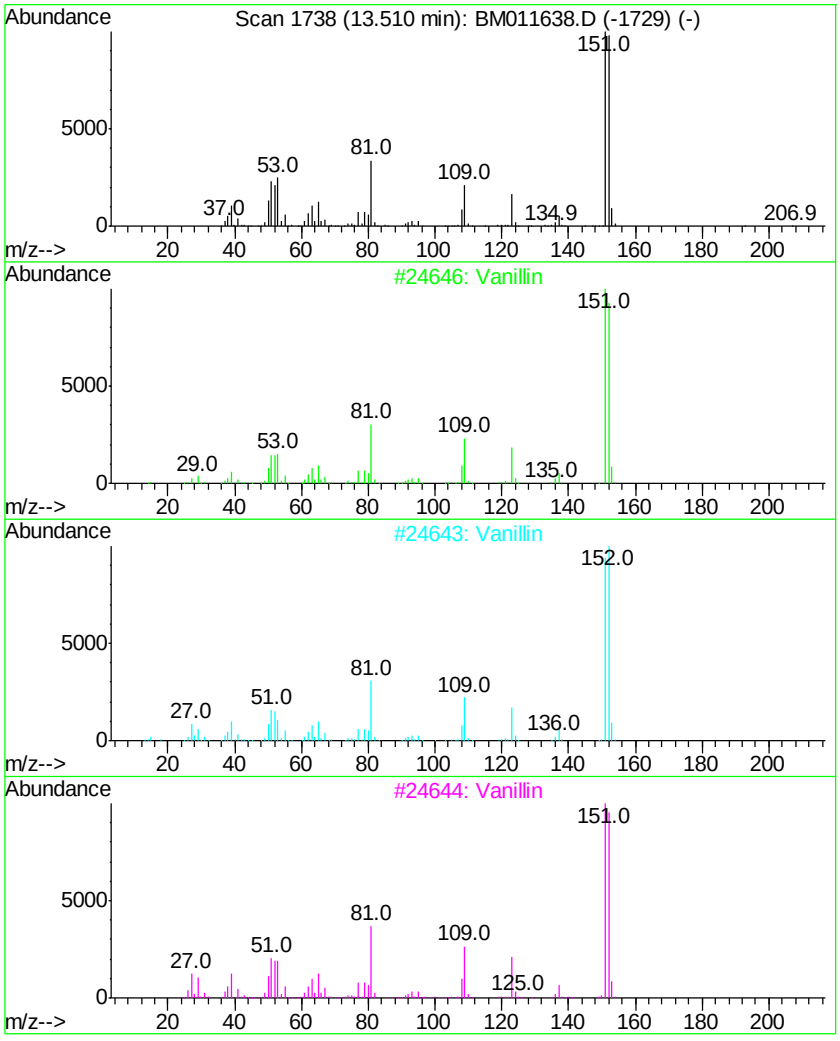
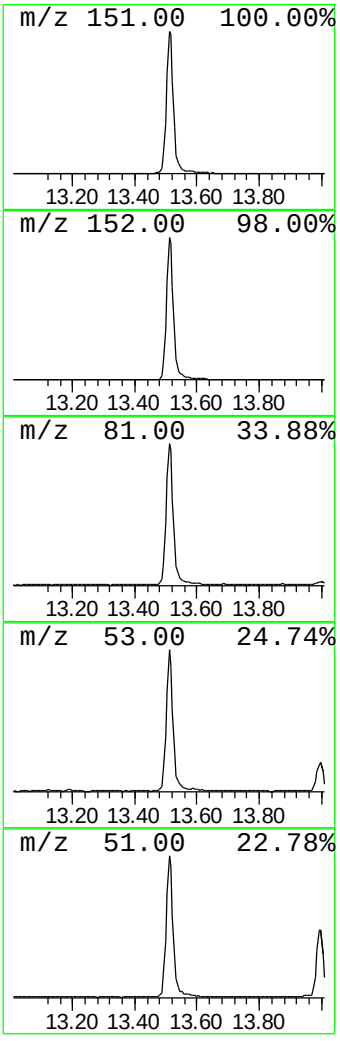
Peak Number 7 Vanillin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	10.24 ng/ul	2499740	Acenaphthene-d10	14.59

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	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94





Library Search Compound Report

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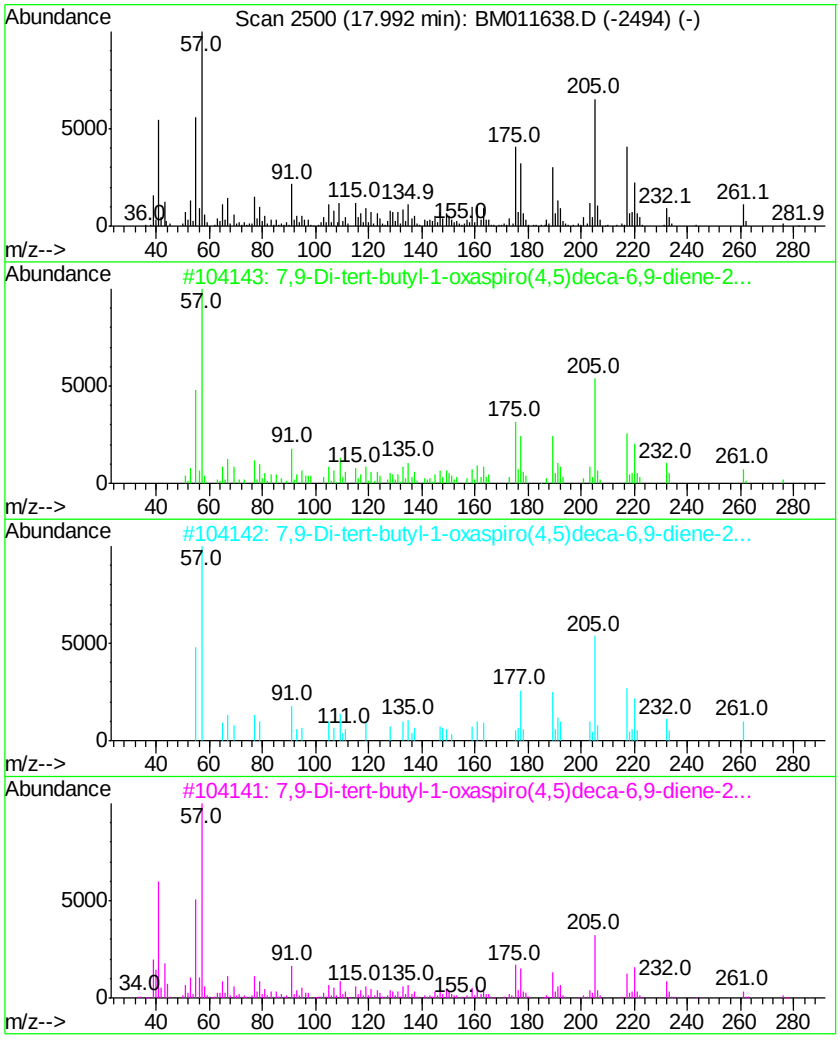
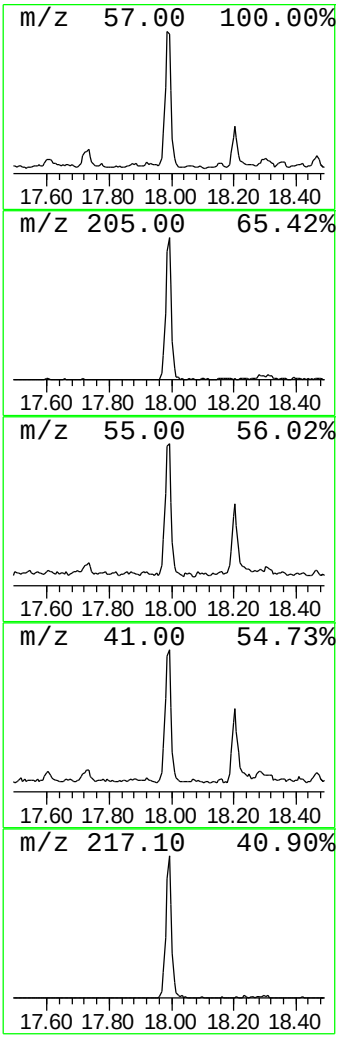
Peak Number 8 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	4.12 ng/ul	1209010	Phenanthrene-d10	17.33

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	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	92
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	70
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	42
5	2,6-Bis(1,1-dimethylethyl)-4-met...	262	C18H30O	004278-82-4	35





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ClientSampleId : C0AC6

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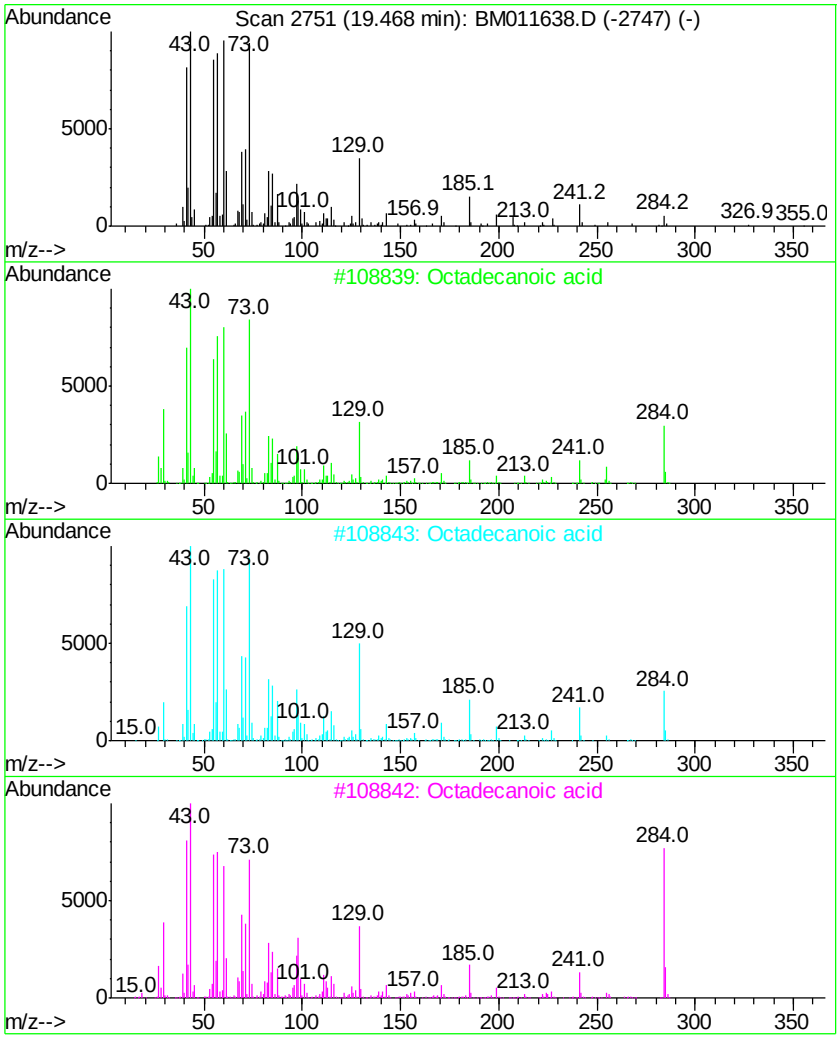
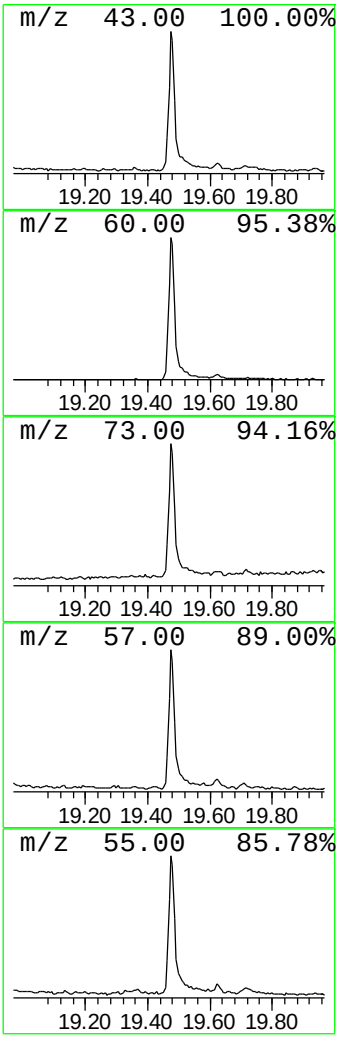
Peak Number 9 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.47	3.19 ng/ul	1048210	Chrysene-d12	21.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	90





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Quant Title : SVOA CALIBRATION

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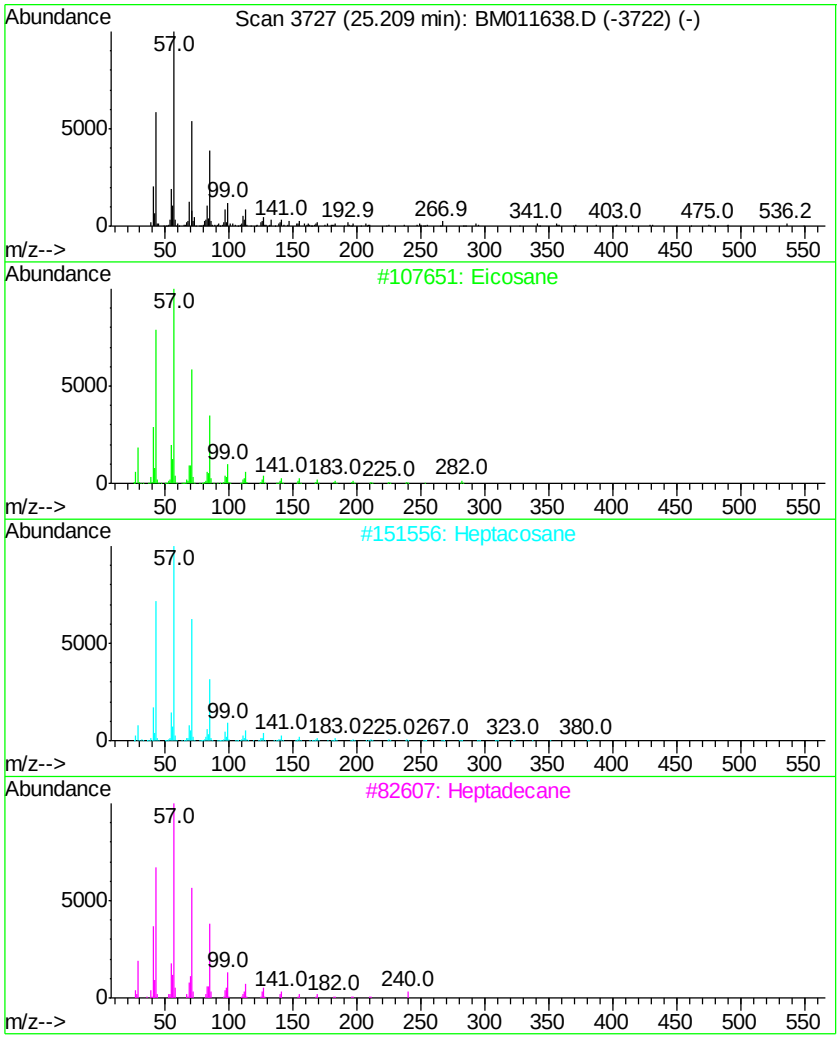
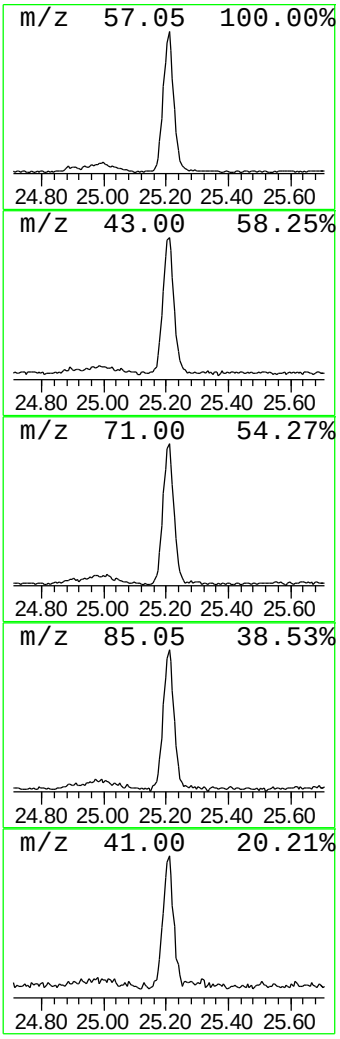
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.21	2.13 ng/ul	617838	Perylene-d12	23.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Heptacosane	380	C27H56	000593-49-7	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	83
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	83





Tentatively Identified Compound (LSC) summary

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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	6.00	34.2	ng/ul	3978430	1	7.96	2323670	20.0
1-Hexanol, 2-ethyl-	8.02	7.0	ng/ul	809877	1	7.96	2323670	20.0
Phenol, 2-methoxy-	9.06	8.8	ng/ul	1017840	1	7.96	2323670	20.0
Ethanol, 2-(hexyl...	9.28	2.1	ng/ul	249684	1	7.96	2323670	20.0
1-(2-Thienyl)-1-p...	10.67	3.0	ng/ul	535416	2	10.77	3549630	20.0
Vanillin	13.51	10.2	ng/ul	2499740	3	14.59	4881110	20.0
7,9-Di-tert-butyl...	17.99	4.1	ng/ul	1209010	4	17.33	5865610	20.0
Octadecanoic acid	19.47	3.2	ng/ul	1048210	5	21.50	6582200	20.0
(DEL) Alkane: Str...	25.21	2.1	ng/ul	617838	6	23.87	5796330	20.0