LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112119\
Data File : BM023830.D
Acq On : 21 Nov 2019 15:43
Operator : JU
Sample : K5851-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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\SOM-EPA-BM111119MA.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	3.057	26	29	39	rVB	47679	75870	1.20%	0.109%
2	3.463	95	98	101	rVB2	14237	16687	0.26%	0.024%
3	3.557	110	114	123	rVB	104844	149332	2.37%	0.214%
4	3.628	123	126	129	rBV4	10865	15840	0.25%	0.023%
5	3.675	129	134	140	rVB	41851	69387	1.10%	0.100%
6	3.757	146	148	153	rVB2	19184	25304	0.40%	0.036%
7	4.310	239	242	248	rVB4	12894	16627	0.26%	0.024%
8	4.669	299	303	307	rBV	45102	74031	1.17%	0.106%
9	4.799	322	325	330	rBV5	7337	10122	0.16%	0.015%
10	5.034	363	365	368	rBV4	5391	7854	0.12%	0.011%
11	5.187	388	391	393	rBV4	4760	6815	0.11%	0.010%
12	5.387	424	425	430	rBV4	4922	7245	0.11%	0.010%
13	5.557	446	454	458	rBV9	8449	16188	0.26%	0.023%
14	5.734	482	484	489	rVB6	6783	8719	0.14%	0.013%
15	5.916	510	515	518	rBV7	4225	8228	0.13%	0.012%
16	6.140	548	553	556	rBV7	8836	13334	0.21%	0.019%
17	6.193	560	562	567	rVV6	4568	8272	0.13%	0.012%
18	6.269	571	575	579	rVB5	10942	16529	0.26%	0.024%
19	6.387	590	595	602	rVB2	34149	52312	0.83%	0.075%
20	6.704	639	649	664	rBV	837755	1441492	22.87%	2.068%
21	6.857	670	675	692	rVB	648608	1082519	17.18%	1.553%
22	7.051	701	708	721	rVV	910549	1473525	23.38%	2.114%
23	7.157	721	726	732	rVB9	12077	23773	0.38%	0.034%
24	7.281	742	747	748	rBV5	6151	8524	0.14%	0.012%
25	7.510	779	786	797	rBV	1165282	1841243	29.21%	2.641%
26	7.934	853	858	862	rBV4	4698	8590	0.14%	0.012%
27	8.228	901	908	924	rBV	968412	1604240	25.45%	2.301%
28	8.339	924	927	932	rVV7	9001	17117	0.27%	0.025%
29	8.663	975	982	993	rVV	777490	1308784	20.77%	1.877%
30	8.804	1002	1006	1009	rBV6	6941	10196	0.16%	0.015%
31	9.110	1055	1058	1067	rVB3	16126	27246	0.43%	0.039%
32	9.381	1096	1104	1112	rBV	637688	1069760	16.97%	1.534%
33	9.922	1185	1196	1205	rBV	1054373	1865872	29.60%	2.676%
34	10.010	1205	1211	1221	rVB2	149672	303211	4.81%	0.435%

LSC Area Percent Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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\SOM-EPA-BM111119MA.M
Title : SVOA CALIBRATION

35	10.157	1230	1236	1243	rVB5	18110	35175	0.56%	0.050%
36	10.286	1250	1258	1272	rBV	1546559	2606986	41.36%	3.739%
37	10.433	1275	1283	1288	rBV	693552	1258418	19.97%	1.805%
38	10.486	1288	1292	1301	rVB	219392	385834	6.12%	0.553%
39	11.116	1394	1399	1402	rBV7	5680	8550	0.14%	0.012%
40	11.886	1525	1530	1537	rVB	21349	38045	0.60%	0.055%
41	11.963	1537	1543	1552	rBV7	8950	19204	0.30%	0.028%
42	12.175	1576	1579	1584	rVB6	4269	6769	0.11%	0.010%
43	12.463	1625	1628	1631	rBV5	4751	6545	0.10%	0.009%
44	12.522	1633	1638	1642	rBV4	14661	20182	0.32%	0.029%
45	12.716	1667	1671	1676	rVB7	4679	6895	0.11%	0.010%
46	12.780	1676	1682	1687	rBV2	16794	25248	0.40%	0.036%
47	12.957	1707	1712	1716	rBV6	9596	16844	0.27%	0.024%
48	13.004	1716	1720	1725	rVB6	7911	14428	0.23%	0.021%
49	13.080	1729	1733	1741	rBV3	32699	57111	0.91%	0.082%
50	13.427	1786	1792	1795	rBV8	3243	6380	0.10%	0.009%
51	13.498	1799	1804	1808	rVB7	13273	18016	0.29%	0.026%
52	13.592	1813	1820	1824	rVV	1829070	2576944	40.89%	3.696%
53	13.639	1824	1828	1838	rVV	709159	1002937	15.91%	1.439%
54	13.721	1840	1842	1849	rVB7	7865	12770	0.20%	0.018%
55	13.857	1858	1865	1877	rBV2	2215501	3376966	53.58%	4.844%
56	13.957	1879	1882	1884	rVB4	8709	10404	0.17%	0.015%
57	13.998	1884	1889	1894	rBV7	5883	12482	0.20%	0.018%
58	14.098	1904	1906	1909	rVB3	8699	8356	0.13%	0.012%
59	14.169	1911	1918	1926	rBV	2349921	3524159	55.92%	5.055%
60	14.227	1926	1928	1933	rVB6	7254	11181	0.18%	0.016%
61	14.398	1951	1957	1972	rBV	453213	962536	15.27%	1.381%
62	14.563	1979	1985	1988	rBV6	21165	48452	0.77%	0.069%
63	14.610	1988	1993	1998	rVB2	97379	156784	2.49%	0.225%
64	14.792	2022	2024	2027	rBV4	8114	9227	0.15%	0.013%
65	14.845	2031	2033	2037	rVB4	12091	15128	0.24%	0.022%
66	15.004	2056	2060	2065	rVB2	25471	38260	0.61%	0.055%
67	15.057	2066	2069	2072	rVB4	11207	12038	0.19%	0.017%
68	15.168	2082	2088	2095	rBV	2991446	4273496	67.81%	6.130%
69	15.227	2095	2098	2106	rVV5	27992	49132	0.78%	0.070%
70	15.310	2106	2112	2122	rVV	550289	841597	13.35%	1.207%
71	15.410	2123	2129	2134	rVB2	37653	61524	0.98%	0.088%

LSC Area Percent Report

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Data File : BM023830.D
Acq On : 21 Nov 2019 15:43
Operator : JU
Sample : K5851-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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\SOM-EPA-BM111119MA.M
Title : SVOA CALIBRATION

72	15.615	2161	2164	2169	rVB6	7882	11602	0.18%	0.017%
73	15.751	2186	2187	2190	rBV3	9271	6923	0.11%	0.010%
74	15.921	2214	2216	2218	rVV3	10811	8512	0.14%	0.012%
75	15.951	2218	2221	2229	rVB10	21975	41326	0.66%	0.059%
76	16.086	2241	2244	2249	rBV7	11732	13741	0.22%	0.020%
77	16.145	2249	2254	2267	rBV	300490	525090	8.33%	0.753%
78	16.357	2287	2290	2292	rBV4	12659	15754	0.25%	0.023%
79	16.580	2325	2328	2330	rBV4	12845	18552	0.29%	0.027%
80	16.657	2339	2341	2344	rBV3	10905	12341	0.20%	0.018%
81	16.710	2347	2350	2353	rBV2	26535	34701	0.55%	0.050%
82	16.851	2371	2374	2376	rBV3	14407	20432	0.32%	0.029%
83	16.921	2380	2386	2391	rVV	2991716	4225199	67.04%	6.060%
84	16.962	2391	2393	2397	rVV	268451	328962	5.22%	0.472%
85	17.021	2397	2403	2414	rVB	3395729	4725926	74.98%	6.779%
86	17.304	2449	2451	2452	rBV2	12671	7592	0.12%	0.011%
87	17.333	2452	2456	2461	rBV2	68413	105267	1.67%	0.151%
88	17.727	2518	2523	2527	rBV6	55464	94796	1.50%	0.136%
89	17.845	2539	2543	2552	rBV	506293	769990	12.22%	1.104%
90	18.721	2688	2692	2698	rBV4	86015	162756	2.58%	0.233%
91	18.992	2734	2738	2744	rVB	502926	679732	10.78%	0.975%
92	19.139	2759	2763	2768	rBV4	156471	239341	3.80%	0.343%
93	19.327	2789	2795	2806	rBV2	4095829	6302601	100.00%	9.040%
94	20.868	3054	3057	3062	rVB	592343	693188	11.00%	0.994%
95	21.127	3096	3101	3105	rBV	3966878	5078694	80.58%	7.285%
96	22.297	3297	3300	3304	rVB	649142	800651	12.70%	1.148%
97	23.144	3439	3444	3450	rBV	3204704	5310540	84.26%	7.617%
98	23.280	3462	3467	3480	rVB	3002976	5265049	83.54%	7.552%

Sum of corrected areas: 69719049

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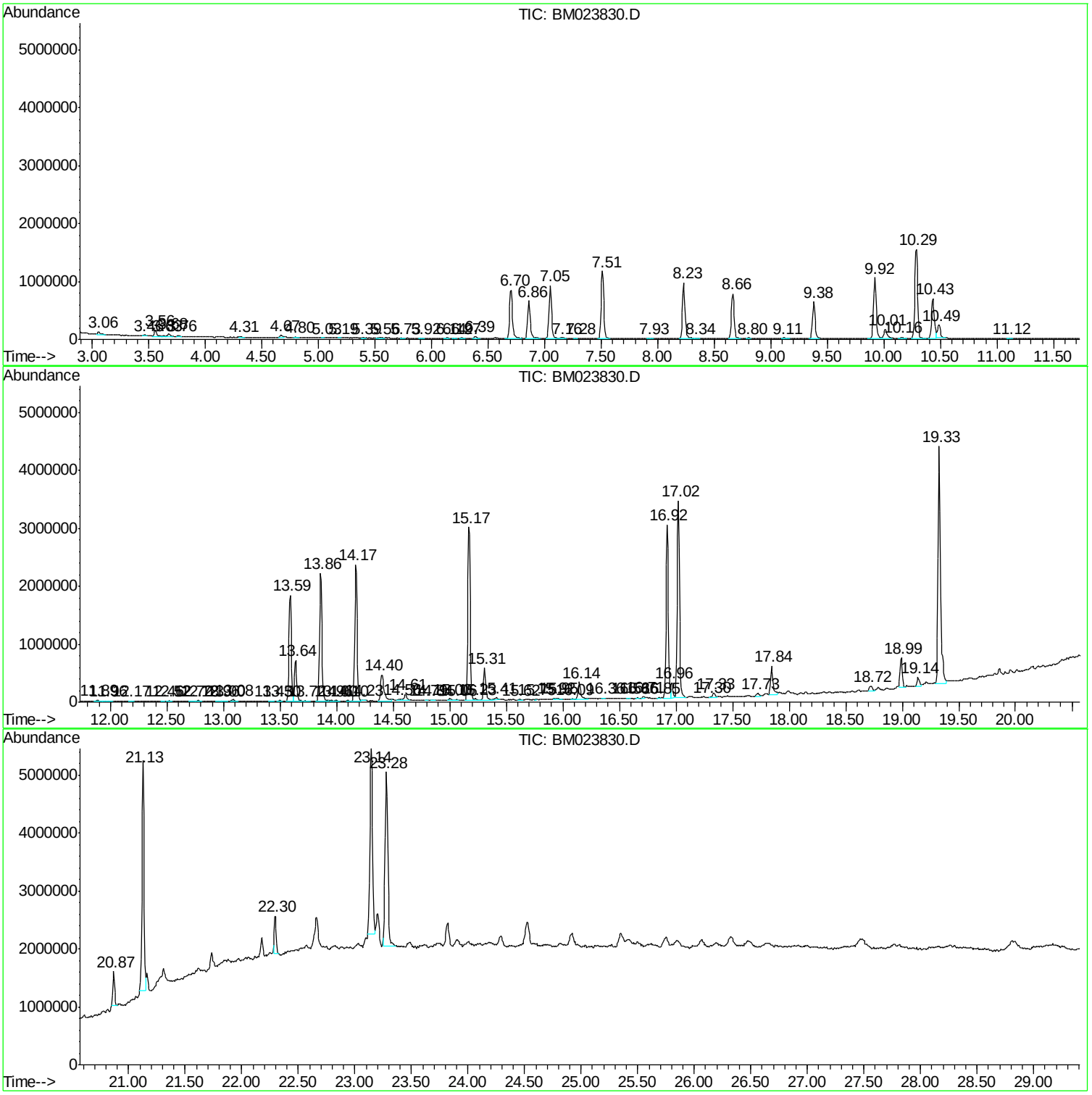
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111119MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112119\
Data File : BM023830.D
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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

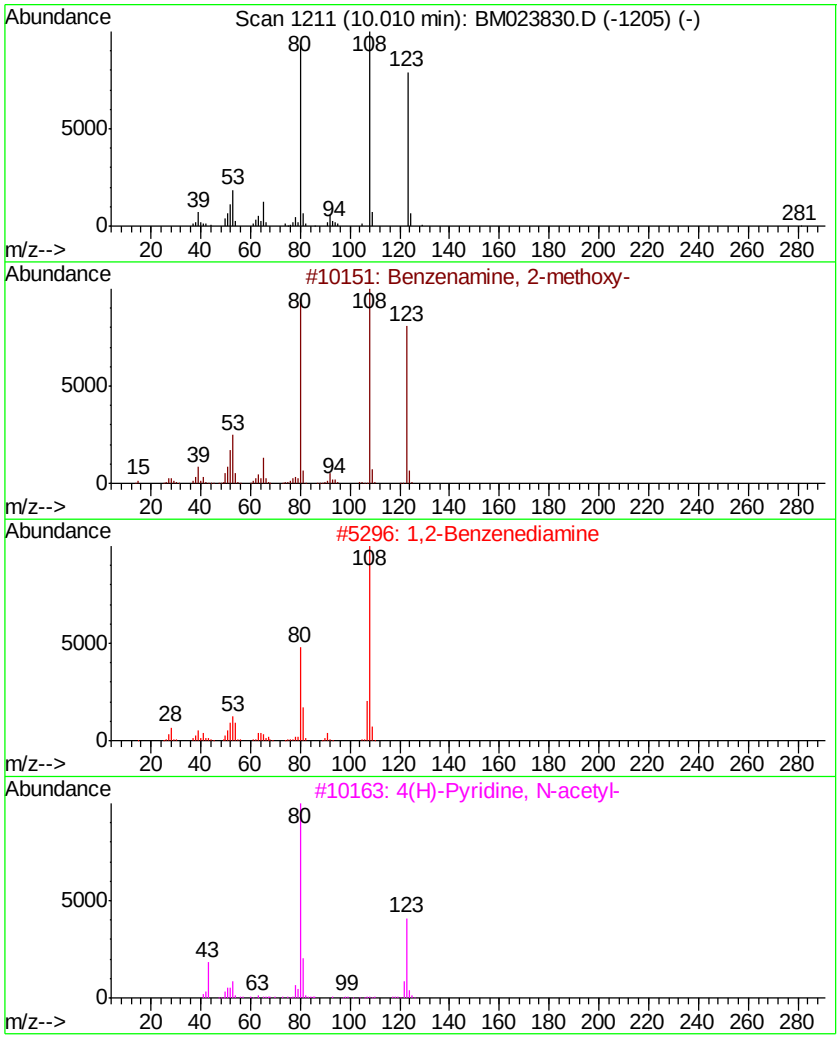
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

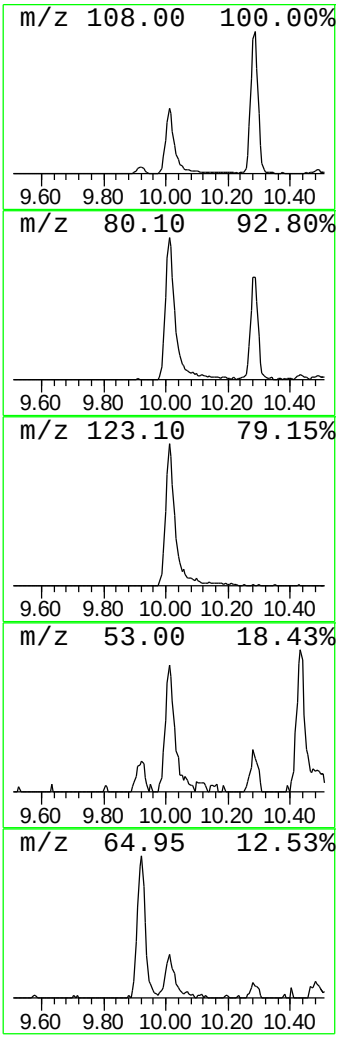
****

Peak Number 1 Benzenamine, 2-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.01	2.33 ng/ul	303211	Naphthalene-d8	10.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2-methoxy-	123	C7H9NO	000090-04-0	95
2	1,2-Benzenediamine	108	C6H8N2	000095-54-5	72
3	4(H)-Pyridine, N-acetyl-	123	C7H9NO	067402-83-9	64
4	Pyrazinamide	123	C5H5N3O	000098-96-4	64
5	2-Pyridinamine, 4-methyl-	108	C6H8N2	000695-34-1	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112119\
Data File : BM023830.D
Acq On : 21 Nov 2019 15:43
Operator : JU
Sample : K5851-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111119MA.M
Quant Title : SVOA CALIBRATION

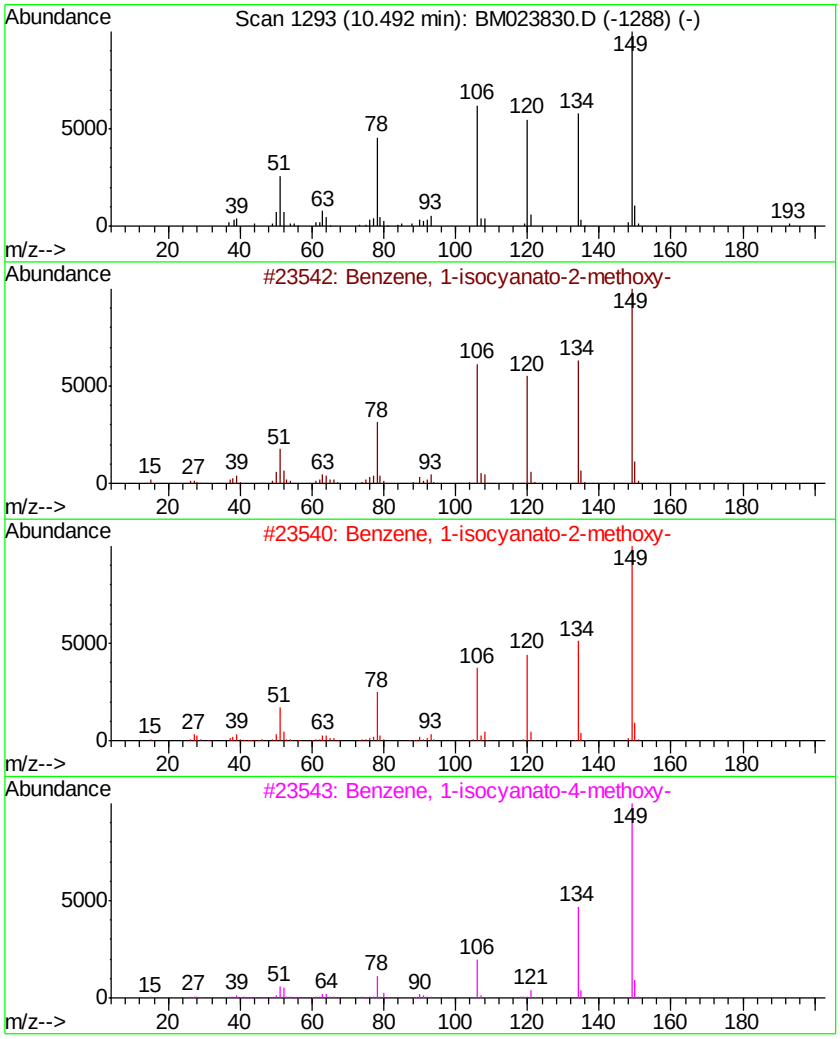
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

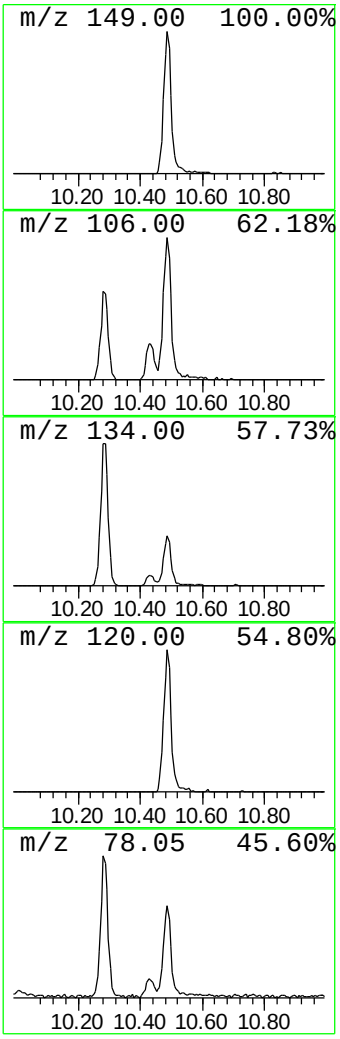
****

Peak Number 2 Benzene, 1-isocyanato-2-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.49	2.96 ng/ul	385834	Naphthalene-d8	10.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	93
2	Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	81
3	Benzene, 1-isocyanato-4-methoxy-	149	C8H7NO2	005416-93-3	49
4	1H-Benzotriazole, 4-methoxy-	149	C7H7N3O	027799-90-2	49
5	1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	46





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Sample : K5851-05
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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111119MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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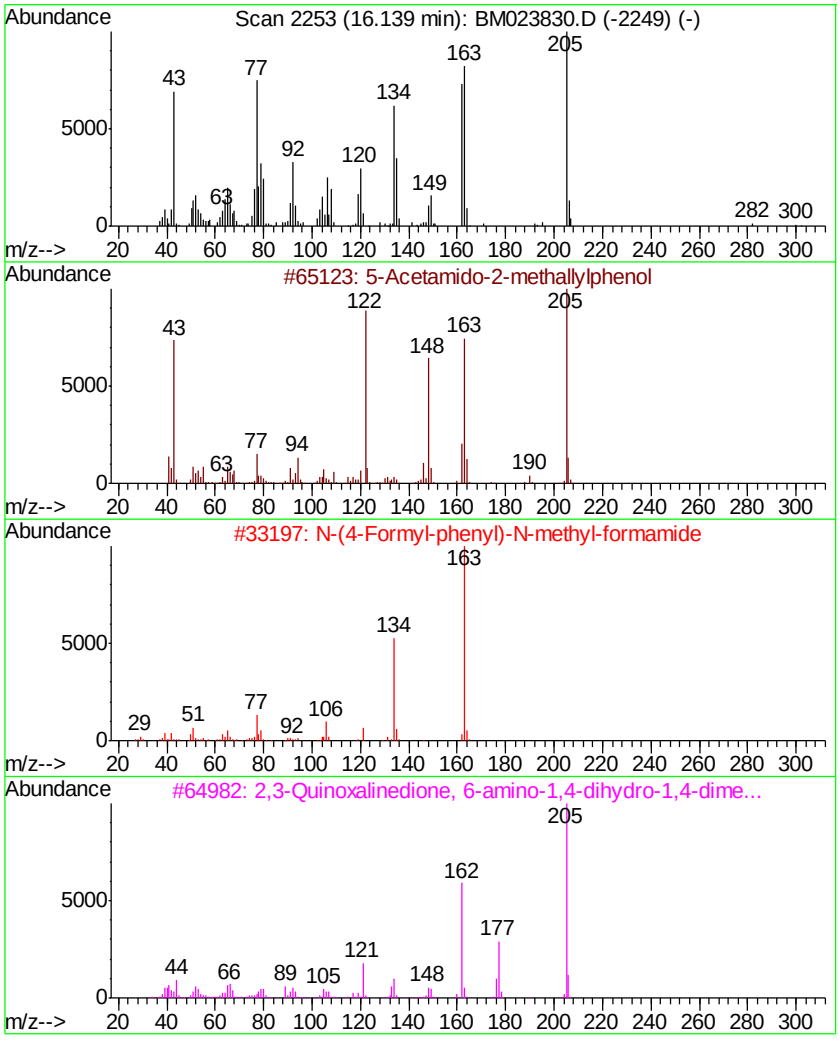
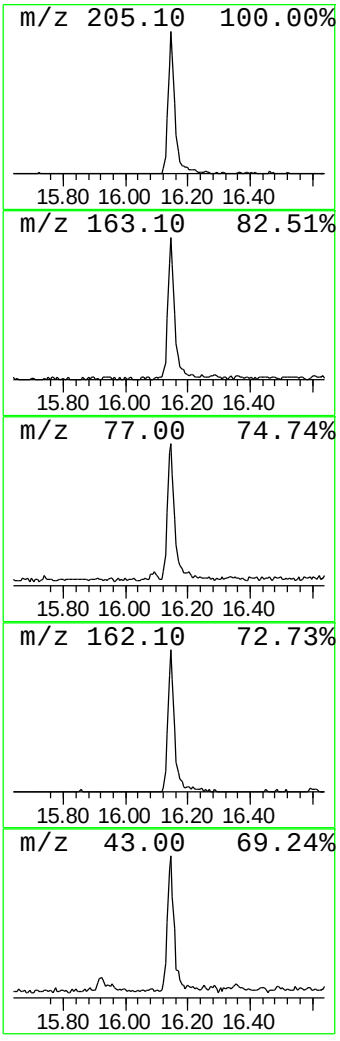
Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	2.49 ng/ul	525090	Phenanthrene-d10	16.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Acetamido-2-methallylphenol	205	C12H15NO2	088913-21-7	43
2	N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	38
3	2,3-Quinoxalinedione, 6-amino-1,...	205	C10H11N3O2	1000338-06-6	35
4	2H-1-Benzopyran-2-one, 3,4-dihyd...	162	C10H10O2	000092-47-7	30
5	1-(4-Methyl-2-pyridyl)-1-propano...	206	C10H14N4O	099171-51-4	30





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111119MA.M
Quant Title : SVOA CALIBRATION

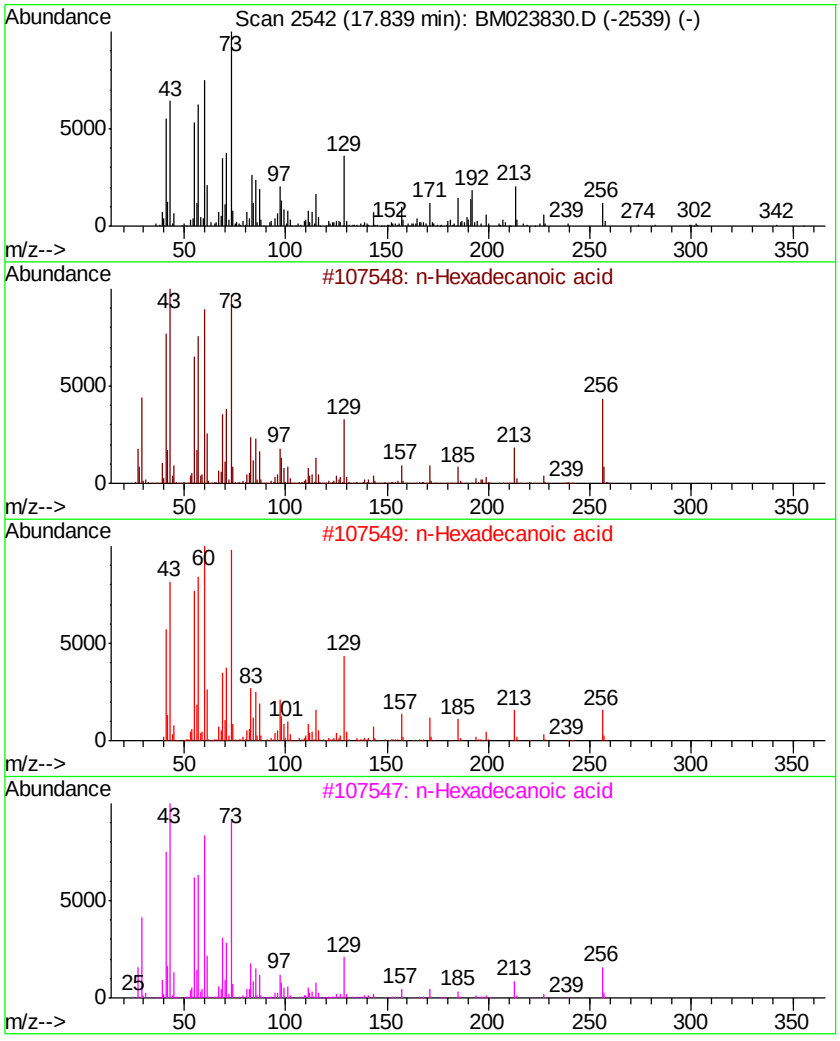
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

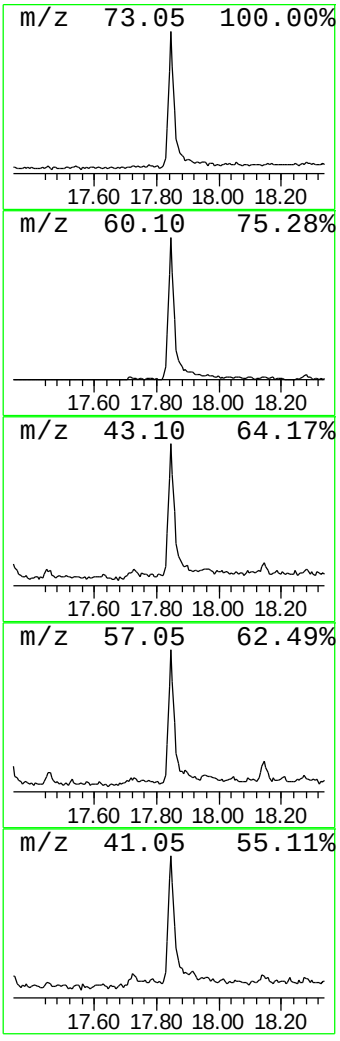
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	3.64 ng/ul	769990	Phenanthrene-d10	16.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4	Octadecanoic acid	284	C18H36O2	000057-11-4	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Data File : BM023830.D
Acq On : 21 Nov 2019 15:43
Operator : JU
Sample : K5851-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111119MA.M
Quant Title : SVOA CALIBRATION

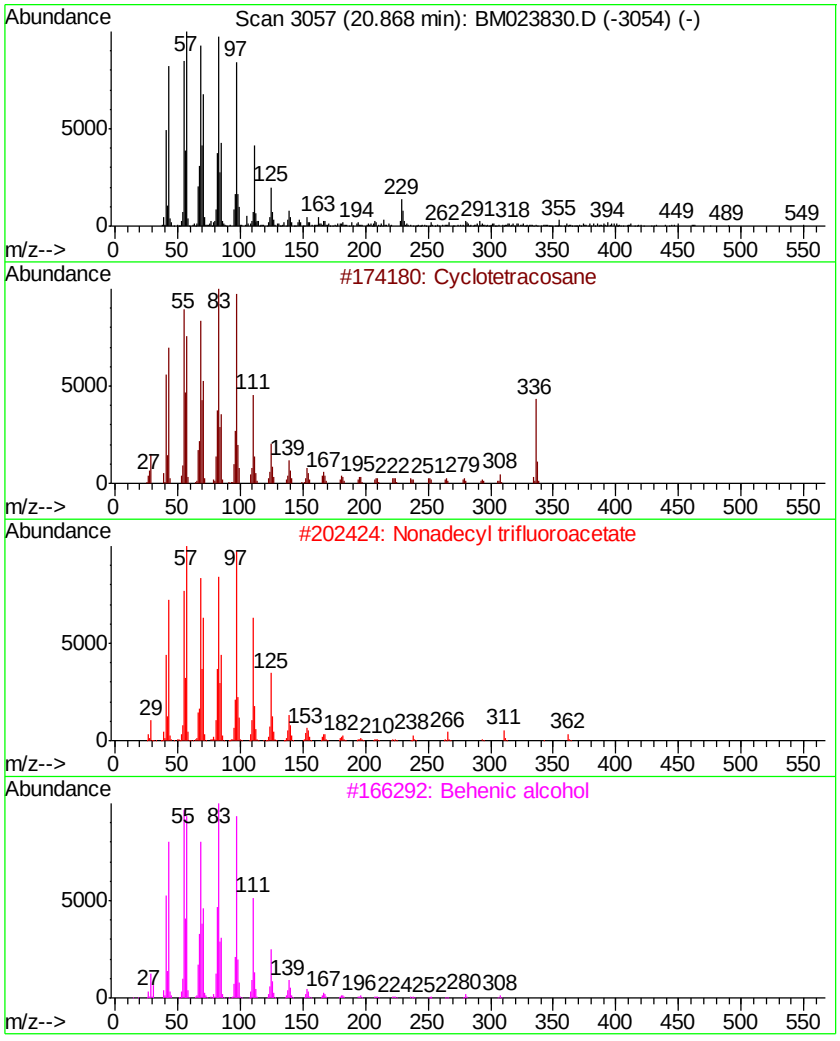
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

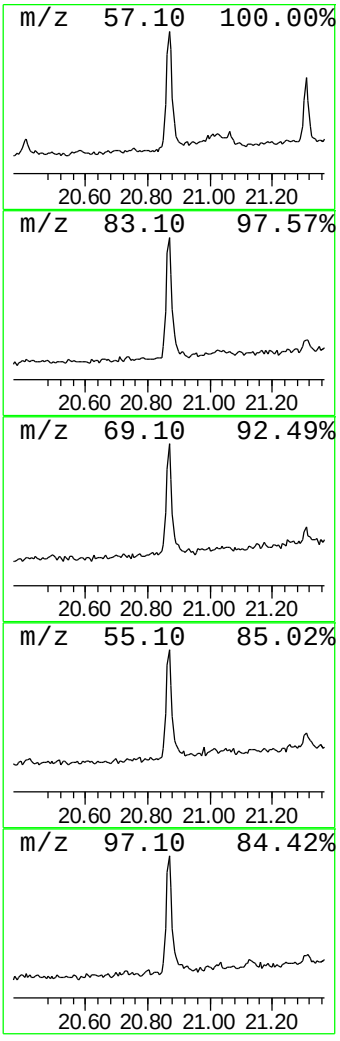
****

Peak Number 5 (DEL) Alkane: Cyclic20.87 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	2.73 ng/ul	693188	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	92





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111119MA.M
Quant Title : SVOA CALIBRATION

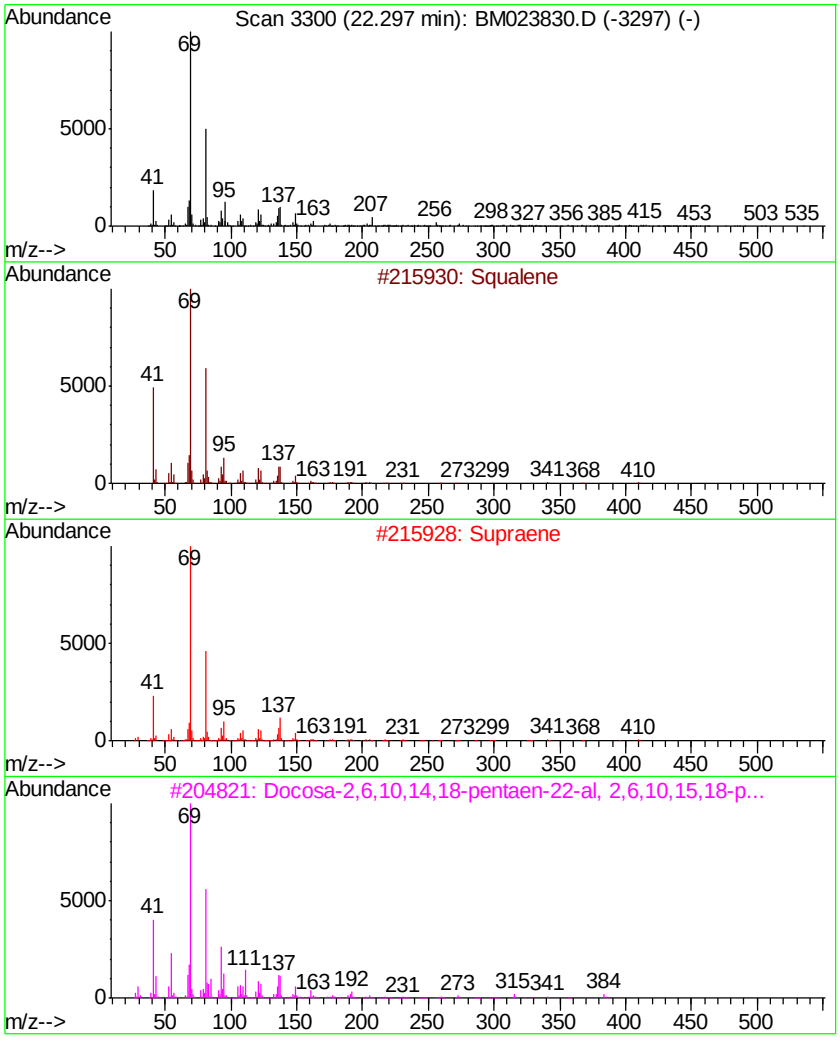
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

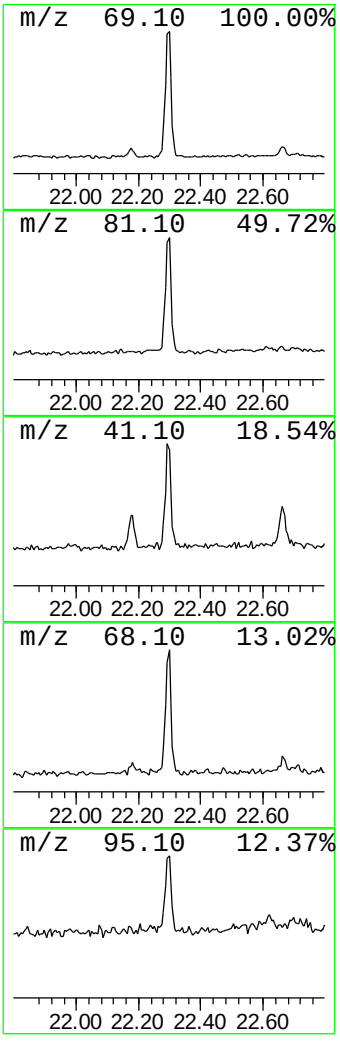
****

Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.30	3.04 ng/ul	800651	Perylene-d12	23.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	83
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	76
5	2,6-Octadiene, 1-(2-bromophenoxy...	308	C16H21BrO	1000163-04-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM112119\
Data File : BM023830.D
Acq On : 21 Nov 2019 15:43
Operator : JU
Sample : K5851-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM111119MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzenamine, 2-me...	10.01	2.3	ng/ul	303211	2	10.29	2606990	20.0
Benzene, 1-isocya...	10.49	3.0	ng/ul	385834	2	10.29	2606990	20.0
unknown-01	16.14	2.5	ng/ul	525090	4	16.92	4225200	20.0
n-Hexadecanoic acid	17.84	3.6	ng/ul	769990	4	16.92	4225200	20.0
(DEL) Alkane: Cyc...	20.87	2.7	ng/ul	693188	5	21.13	5078690	20.0
Squalene	22.30	3.0	ng/ul	800651	6	23.28	5265050	20.0