LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
Data File : BM018572.D
Acq On : 15 Jan 2019 21:53
Operator : JU/SJ
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BM010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.628	72	92	102	rBV2	412788	2241550	6.98%	0.805%
2	4.334	138	212	216	rBV3	2809539	32126465	100.00%	11.543%
3	4.946	304	316	320	rBV	1429411	4055183	12.62%	1.457%
4	5.105	328	343	345	rVB2	790337	2439036	7.59%	0.876%
5	5.281	363	373	379	rBV2	336129	645190	2.01%	0.232%
6	5.346	379	384	390	rVV	1074515	1938767	6.03%	0.697%
7	5.510	390	412	415	rVB	948874	4778134	14.87%	1.717%
8	5.869	467	473	481	rVB	910533	1499733	4.67%	0.539%
9	6.157	514	522	527	rBV	2773609	4624729	14.40%	1.662%
10	6.940	624	655	657	rBV2	1792602	7045403	21.93%	2.531%
11	7.293	711	715	721	rBV	1941561	3716233	11.57%	1.335%
12	7.551	755	759	766	rVB	1046828	1726571	5.37%	0.620%
13	7.751	786	793	796	rBV	667648	1145399	3.57%	0.412%
14	7.793	796	800	803	rVV	775940	1151693	3.58%	0.414%
15	7.934	817	824	829	rVB	397138	709404	2.21%	0.255%
16	8.028	829	840	844	rBV2	1818978	4344682	13.52%	1.561%
17	8.075	844	848	854	rVV2	1924489	3306013	10.29%	1.188%
18	8.204	865	870	880	rBV2	645303	1315433	4.09%	0.473%
19	8.534	905	926	931	rBV	3134532	10692562	33.28%	3.842%
20	8.922	985	992	999	rVB	1403708	2432627	7.57%	0.874%
21	9.275	1020	1052	1055	rBV	2777870	15935559	49.60%	5.726%
22	9.375	1064	1069	1073	rBV	555549	769136	2.39%	0.276%
23	9.728	1121	1129	1133	rBV	1124160	2156601	6.71%	0.775%
24	10.010	1164	1177	1180	rBV3	2041911	7563793	23.54%	2.718%
25	10.098	1188	1192	1193	rBV2	807017	1179148	3.67%	0.424%
26	10.463	1253	1254	1256	rVB	5044109	1962615	6.11%	0.705%
27	10.492	1257	1259	1263	rVB	519568	590400	1.84%	0.212%
28	10.545	1263	1268	1272	rVB	944175	1494634	4.65%	0.537%
29	10.640	1280	1284	1289	rVB	753085	988936	3.08%	0.355%
30	10.745	1291	1302	1306	rBV3	811022	1708938	5.32%	0.614%
31	10.851	1306	1320	1322	rBV2	5966182	15883828	49.44%	5.707%
32	11.116	1361	1365	1369	rVB	726380	1064355	3.31%	0.382%
33	11.192	1374	1378	1381	rVV	558849	910213	2.83%	0.327%
34	11.239	1381	1386	1390	rVV	752166	1316977	4.10%	0.473%

LSC Area Percent Report

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Sample : K1127-02
Misc :
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Instrument : BNA_M
ClientSampleId : COMP-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.316	1394	1399	1403	rVV	822503	1343444	4.18%	0.483%
36	11.398	1403	1413	1419	rVV3	3524199	7756936	24.15%	2.787%
37	11.498	1419	1430	1432	rVV3	1433021	4302501	13.39%	1.546%
38	11.522	1432	1434	1442	rVB2	1107373	1318001	4.10%	0.474%
39	11.634	1442	1453	1459	rBV2	1166028	2824625	8.79%	1.015%
40	11.810	1477	1483	1487	rBV	2053573	3437622	10.70%	1.235%
41	11.863	1487	1492	1497	rVV	1335410	2300901	7.16%	0.827%
42	11.916	1497	1501	1513	rVB5	375103	1078493	3.36%	0.388%
43	12.022	1513	1519	1527	rBV5	334880	601718	1.87%	0.216%
44	12.104	1529	1533	1539	rBV4	230147	568677	1.77%	0.204%
45	12.175	1539	1545	1548	rBV3	691268	1246342	3.88%	0.448%
46	12.210	1548	1551	1555	rVB3	422406	600877	1.87%	0.216%
47	12.334	1567	1572	1580	rBV4	1448370	3196318	9.95%	1.148%
48	12.563	1606	1611	1613	rVV2	619522	1014537	3.16%	0.365%
49	12.604	1613	1618	1619	rVV2	1148014	1931625	6.01%	0.694%
50	12.628	1619	1622	1632	rVB2	1774165	3485226	10.85%	1.252%
51	12.834	1650	1657	1665	rVB	2260433	3866652	12.04%	1.389%
52	12.928	1665	1673	1679	rBV	506385	984585	3.06%	0.354%
53	13.016	1680	1688	1698	rVB	3879345	7069756	22.01%	2.540%
54	13.151	1705	1711	1714	rBV5	312221	598543	1.86%	0.215%
55	13.204	1714	1720	1729	rVB2	1298715	2793504	8.70%	1.004%
56	13.363	1743	1747	1750	rVB4	347737	523024	1.63%	0.188%
57	13.457	1758	1763	1770	rBV4	399832	889316	2.77%	0.320%
58	13.551	1774	1779	1782	rBV3	726435	1222653	3.81%	0.439%
59	13.598	1784	1787	1792	rVV4	1008408	1611086	5.01%	0.579%
60	13.675	1796	1800	1808	rVB5	451127	1050053	3.27%	0.377%
61	13.869	1829	1833	1836	rVV	746530	999491	3.11%	0.359%
62	13.904	1836	1839	1844	rVB3	726302	924476	2.88%	0.332%
63	13.969	1844	1850	1854	rBV3	824721	1363552	4.24%	0.490%
64	14.045	1859	1863	1867	rVV	1026687	1486803	4.63%	0.534%
65	14.122	1867	1876	1886	rVV4	1151462	4191258	13.05%	1.506%
66	14.198	1887	1889	1892	rVV3	380983	551332	1.72%	0.198%
67	14.251	1893	1898	1900	rVV2	562460	1188377	3.70%	0.427%
68	14.275	1900	1902	1906	rVV2	863594	1240907	3.86%	0.446%
69	14.316	1906	1909	1912	rVV3	394276	596318	1.86%	0.214%
70	14.351	1912	1915	1919	rVV3	384845	728857	2.27%	0.262%
71	14.404	1919	1924	1931	rVB2	1643769	2719392	8.46%	0.977%

LSC Area Percent Report

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Sample : K1127-02
Misc :
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Instrument : BNA_M
ClientSampleId : COMP-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.522	1939	1944	1952	rBV3	479897	1157582	3.60%	0.416%
73	14.604	1955	1958	1965	rVB2	418021	666129	2.07%	0.239%
74	14.686	1967	1972	1978	rBV5	335730	745539	2.32%	0.268%
75	14.745	1978	1982	1984	rVV3	361224	540020	1.68%	0.194%
76	14.775	1984	1987	1992	rVB	569695	787114	2.45%	0.283%
77	15.175	2046	2055	2058	rVV3	844402	1591491	4.95%	0.572%
78	15.216	2058	2062	2065	rBV3	442675	700832	2.18%	0.252%
79	15.386	2088	2091	2095	rVB2	517864	644723	2.01%	0.232%
80	15.433	2095	2099	2110	rVB3	817904	1578548	4.91%	0.567%
81	15.898	2172	2178	2188	rBV	3580148	5223686	16.26%	1.877%
82	16.439	2260	2270	2276	rVB	2044912	5062321	15.76%	1.819%
83	16.504	2277	2281	2287	rBV7	330954	681594	2.12%	0.245%
84	16.780	2324	2328	2341	rVB3	343119	735105	2.29%	0.264%
85	17.151	2386	2391	2401	rVB	2134959	3084307	9.60%	1.108%
86	17.321	2417	2420	2428	rVB4	369115	554154	1.72%	0.199%
87	17.916	2517	2521	2528	rBV	702083	1019116	3.17%	0.366%
88	18.051	2539	2544	2553	rVB	3481607	4900198	15.25%	1.761%
89	18.533	2622	2626	2631	rVB3	397911	576759	1.80%	0.207%
90	18.592	2632	2636	2639	rBV3	435643	718665	2.24%	0.258%
91	18.692	2649	2653	2659	rVB2	526085	760282	2.37%	0.273%
92	19.204	2735	2740	2747	rVB4	685790	1126502	3.51%	0.405%
93	19.327	2757	2761	2769	rVV	1812377	2573006	8.01%	0.924%
94	19.415	2773	2776	2785	rVB	394513	722589	2.25%	0.260%
95	19.780	2833	2838	2847	rBV	7626211	8887593	27.66%	3.193%
96	21.039	3048	3052	3057	rBV	1274873	1468672	4.57%	0.528%
97	21.339	3099	3103	3109	rVB	3256932	4165722	12.97%	1.497%
98	22.515	3299	3303	3311	rVB	2533965	3464604	10.78%	1.245%
99	23.621	3485	3491	3499	rVB2	2305532	4387743	13.66%	1.577%
100	24.903	3704	3709	3716	rVB2	357160	728385	2.27%	0.262%

Sum of corrected areas: 278320699

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
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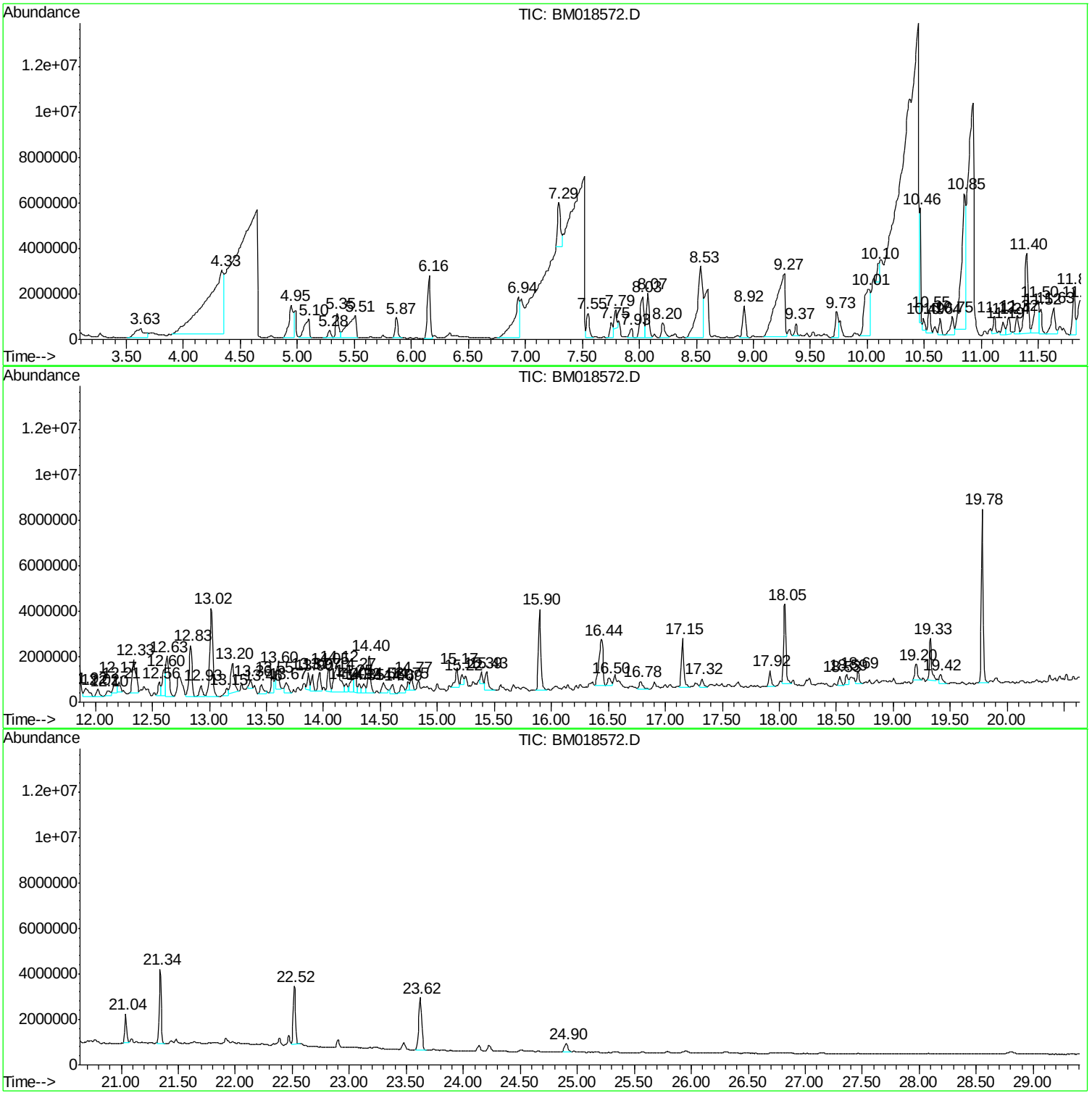
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
Data File : BM018572.D
Acq On : 15 Jan 2019 21:53
Operator : JU/SJ
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

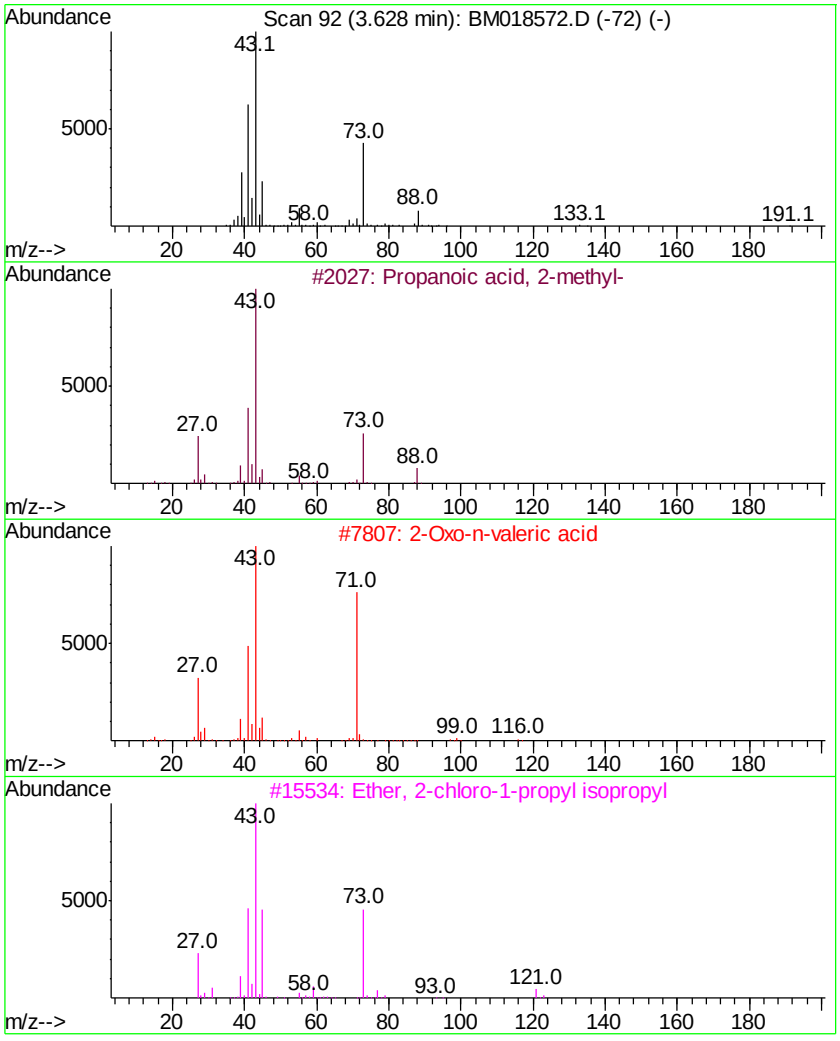
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

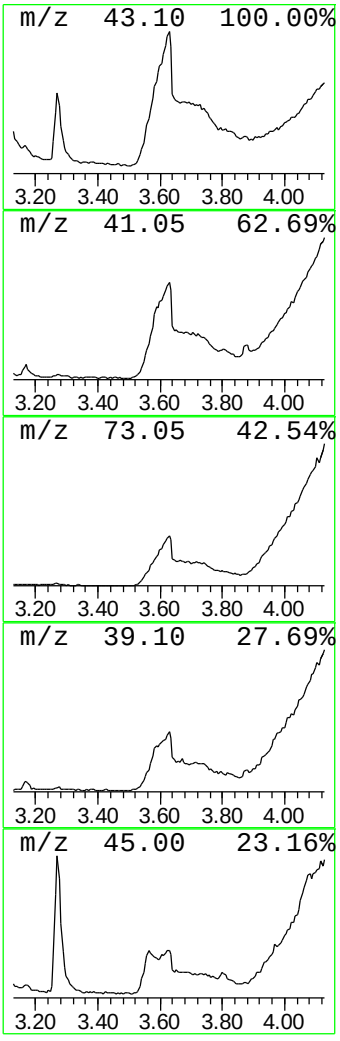
****

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.63	39.14 ng	2241550	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	80
2	2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	23
3	Ether, 2-chloro-1-propyl isopropyl	136	C6H13ClO	1000150-65-2	23
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	23
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	16





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Sample : K1127-02
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Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

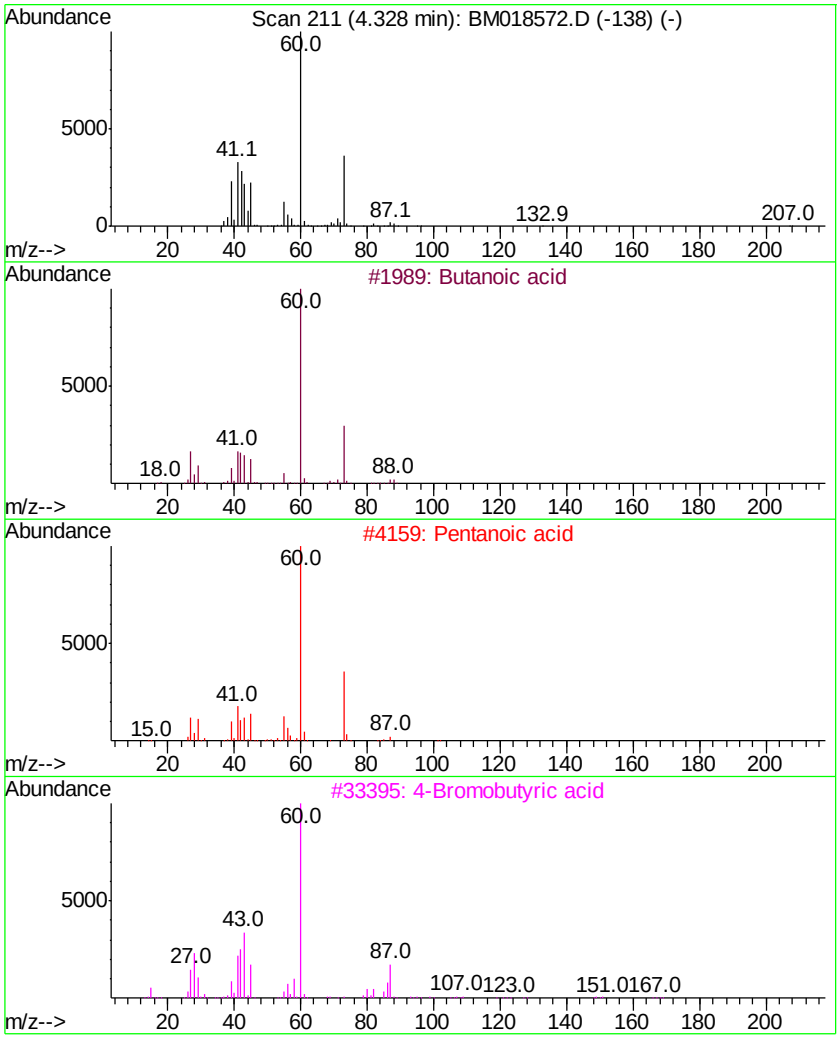
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

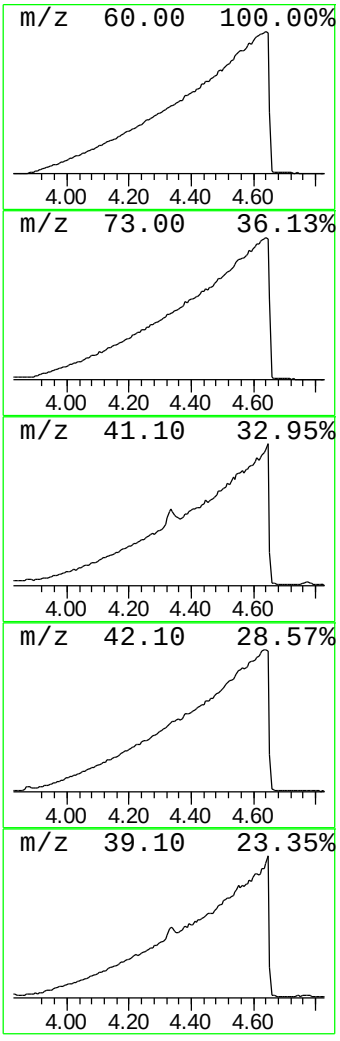
****

Peak Number 2 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	560.97 ng	32126500	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	72
2	Pentanoic acid	102	C5H10O2	000109-52-4	45
3	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	38
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	23
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	11





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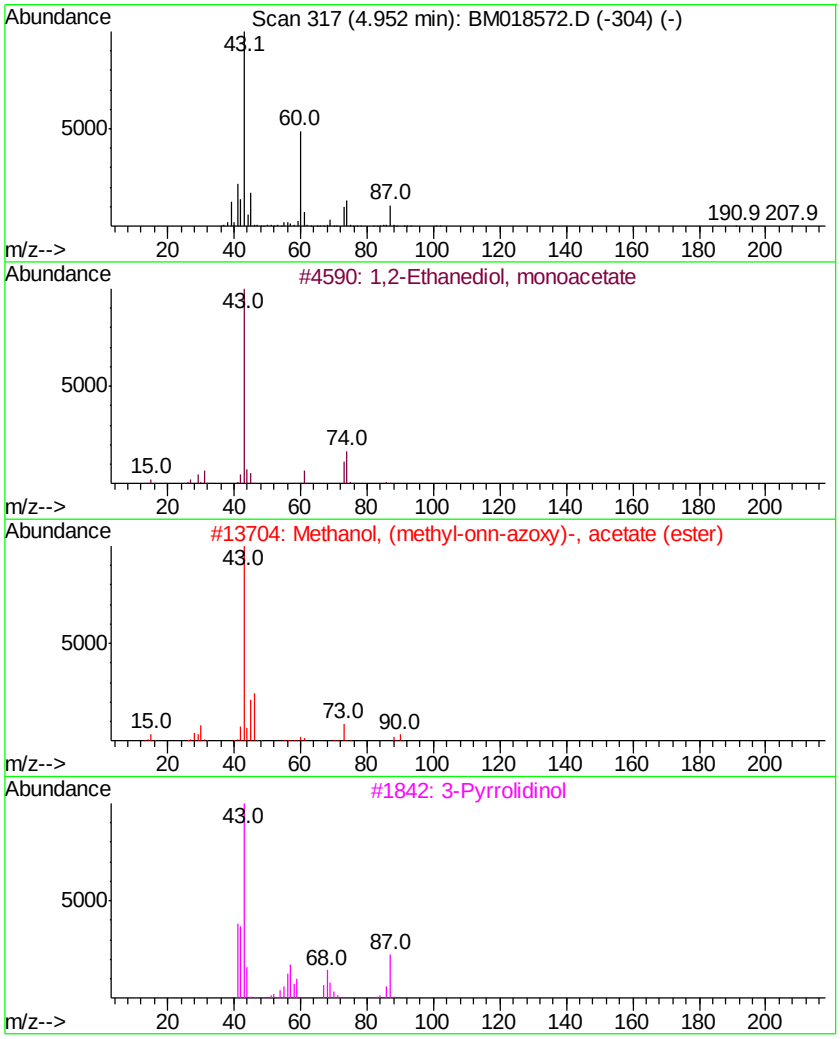
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

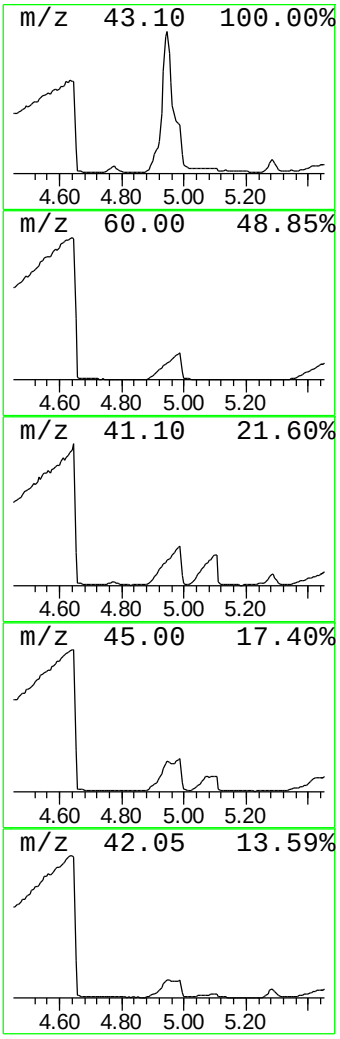
****

Peak Number 3 unknown4.95 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	70.81 ng	4055180	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol, monoacetate	104	C4H8O3	000542-59-6	37
2	Methanol, (methyl-onn-azoxy)-, a...	132	C4H8N2O3	000592-62-1	28
3	3-Pyrrolidinol	87	C4H9NO	040499-83-0	9
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	9





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Data File : BM018572.D
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Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

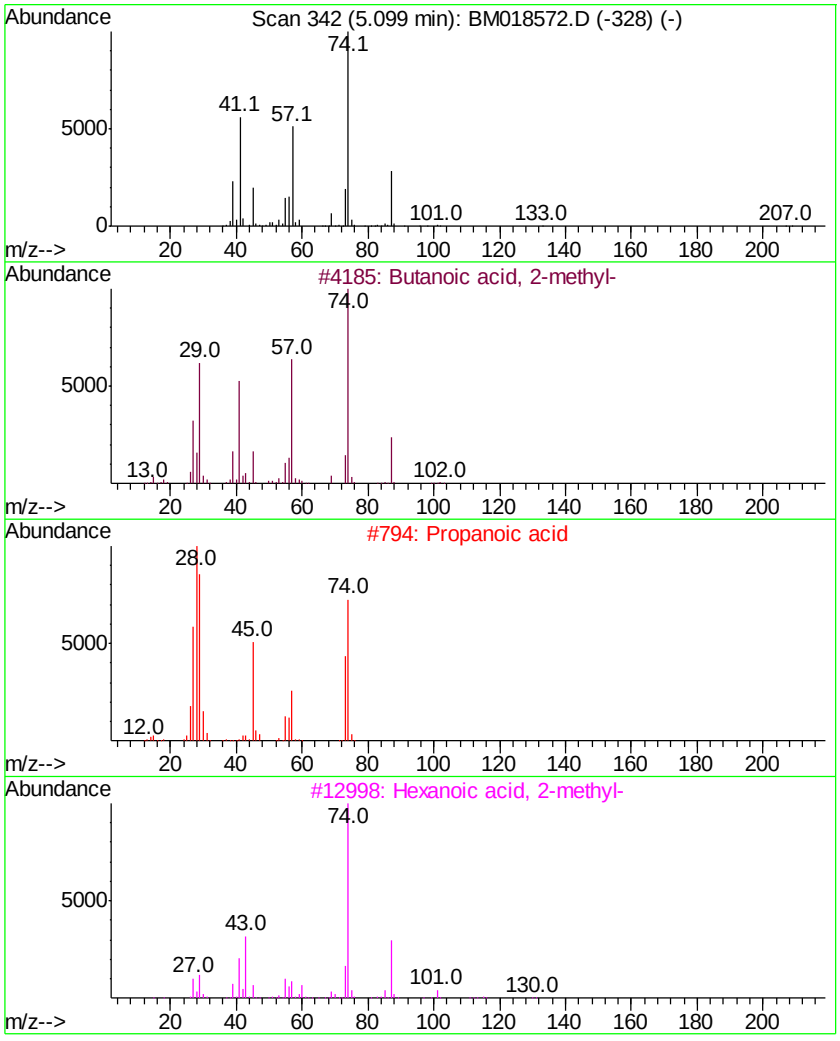
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

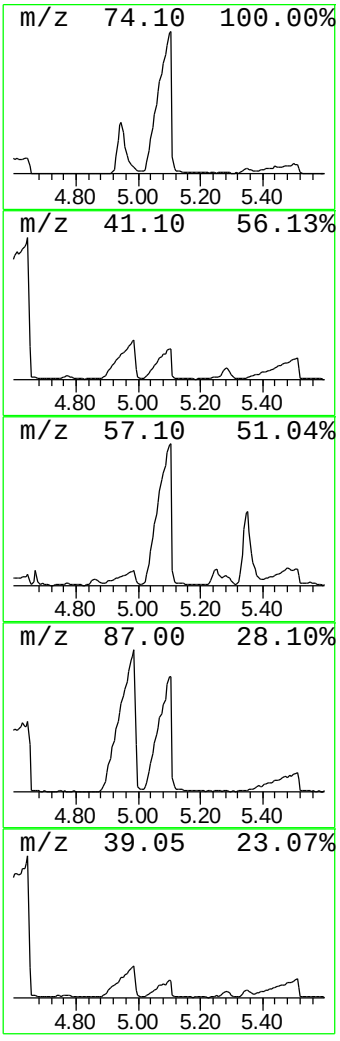
****

Peak Number 4 Butanoic acid, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	42.59 ng	2439040	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
2	Propanoic acid	74	C3H6O2	000079-09-4	38
3	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	38
4	5-Hydroxy-2,2-dimethylhexan-3-one	144	C8H16O2	173343-33-4	10
5	Morpholine	87	C4H9NO	000110-91-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
Data File : BM018572.D
Acq On : 15 Jan 2019 21:53
Operator : JU/SJ
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

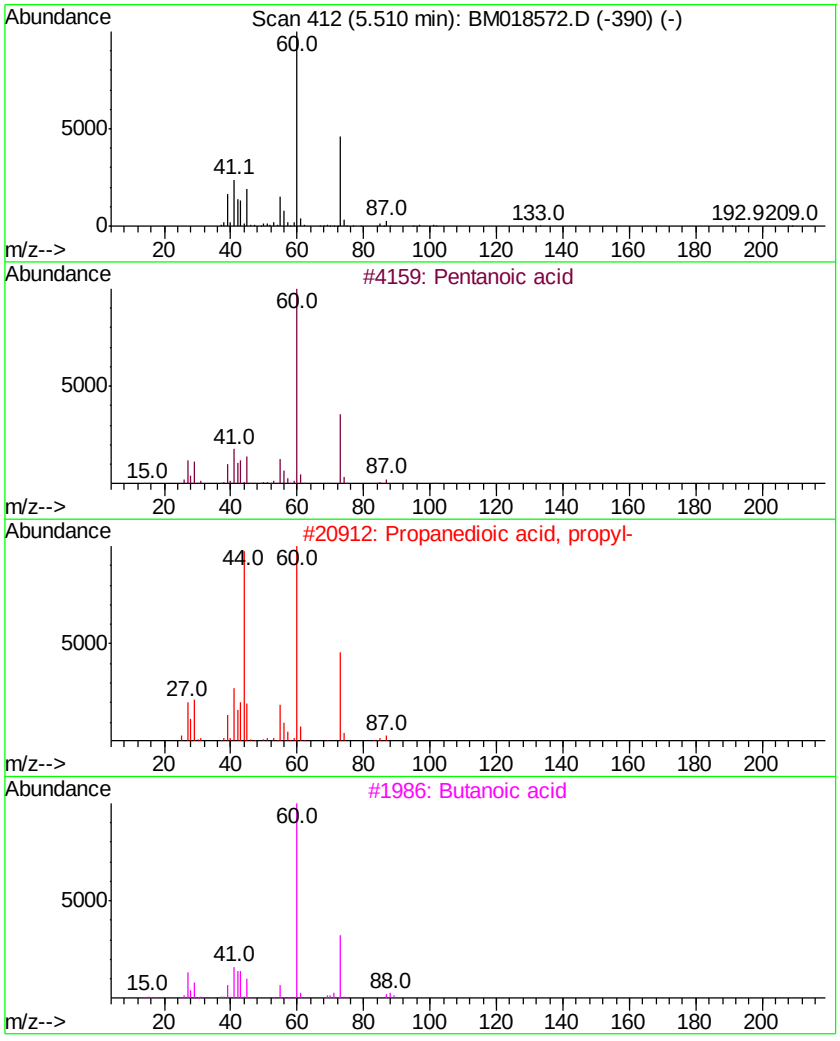
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

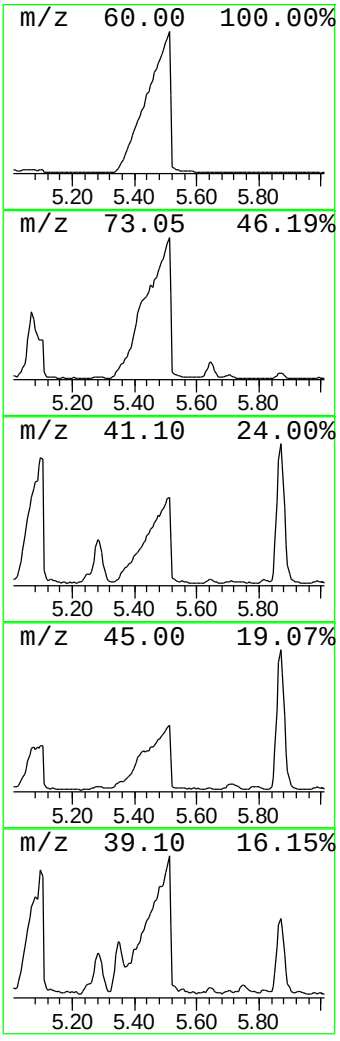
****

Peak Number 5 Pentanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	83.43 ng	4778130	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	78
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	74
3	Butanoic acid	88	C4H8O2	000107-92-6	72
4	Hexanoic acid	116	C6H12O2	000142-62-1	64
5	Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	40





Library Search Compound Report

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Acq On : 15 Jan 2019 21:53
Operator : JU/SJ
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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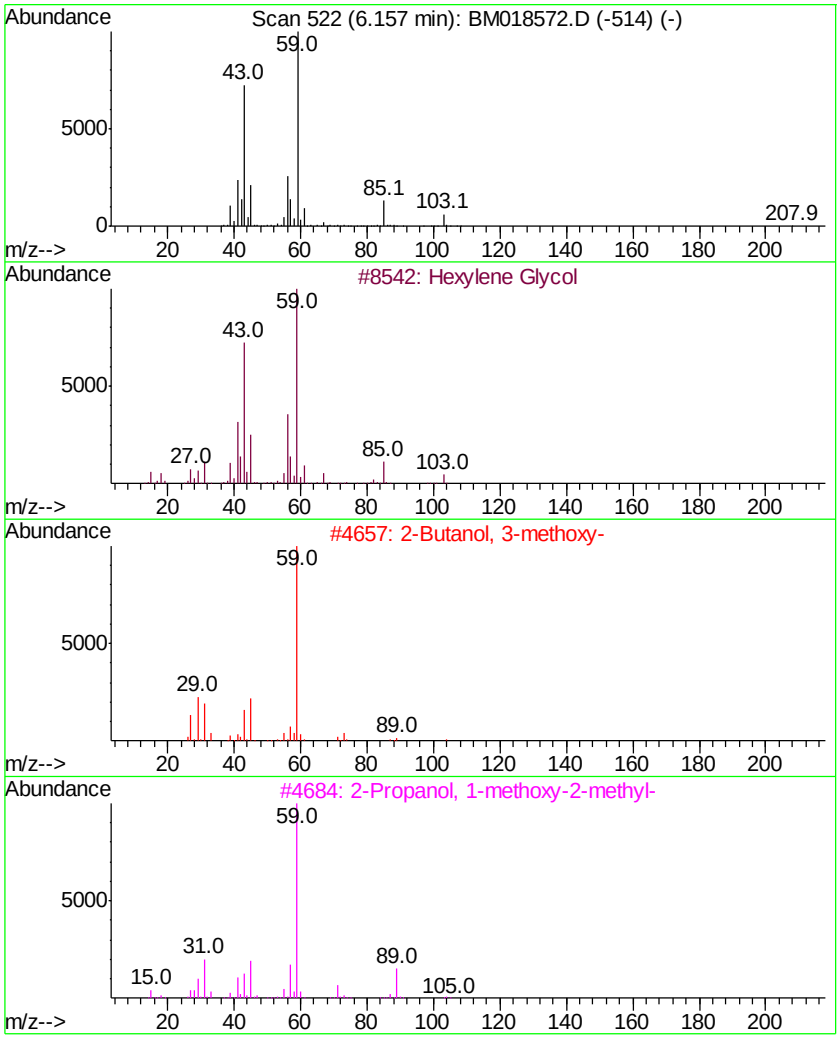
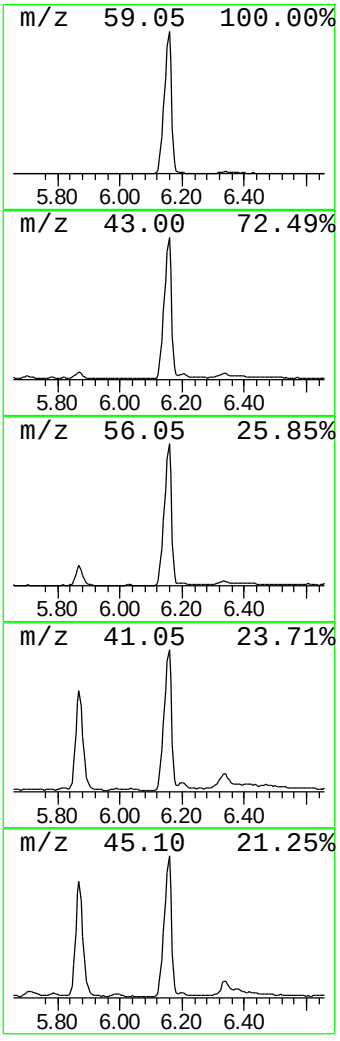
Peak Number 6 Hexylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	80.75 ng	4624730	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene Glycol	118	C6H14O2	000107-41-5	90
2	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	50
3	2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	47
4	Ethanimidic acid, ethyl ester	87	C4H9NO	001000-84-6	47
5	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	45





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Instrument : BNA_M
ClientSampleId : COMP-1

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

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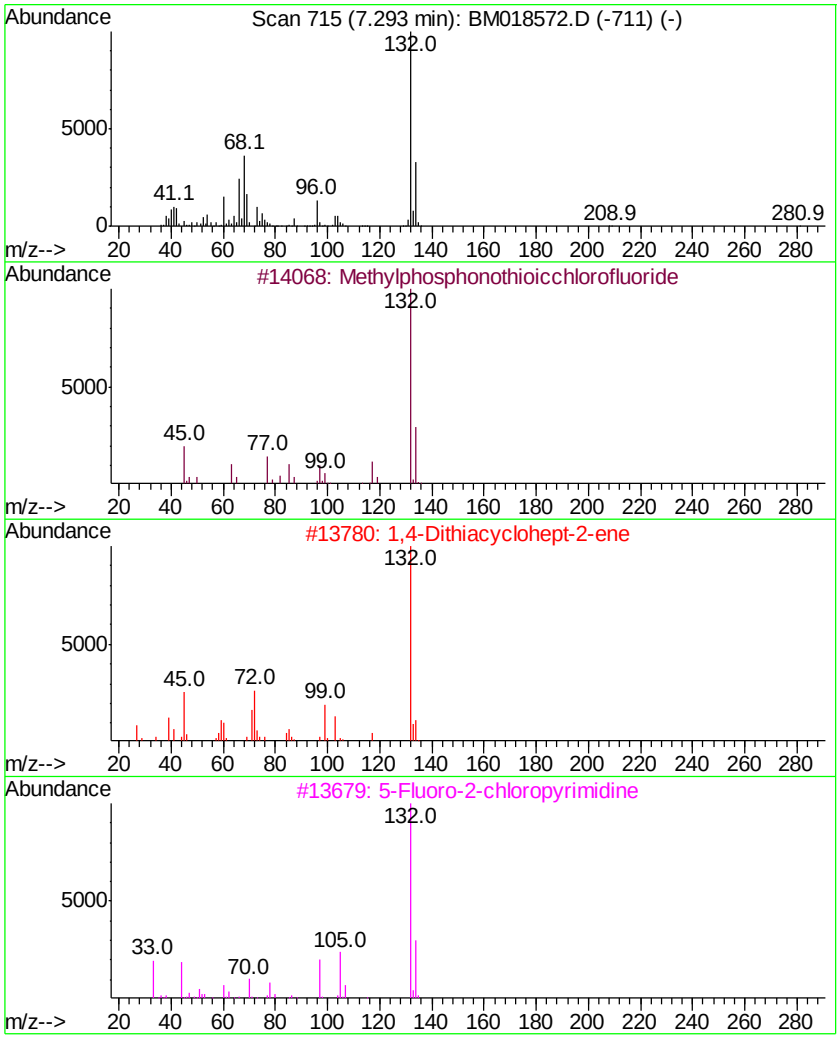
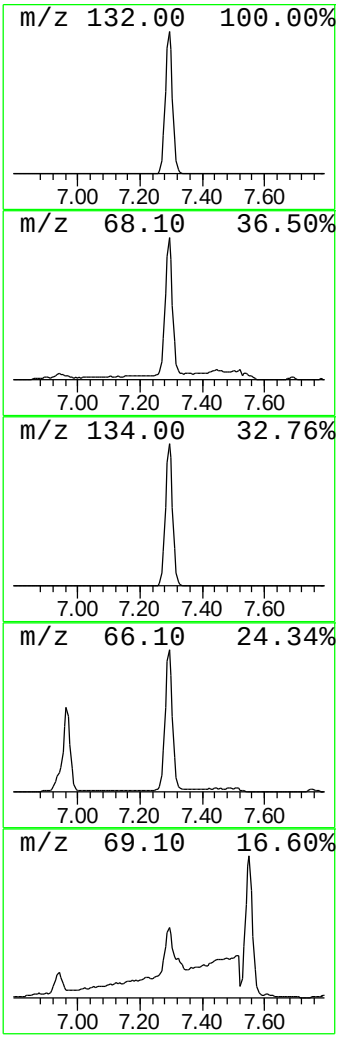
Peak Number 7 unknown7.29 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	64.89 ng	3716230	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylphosphonothioicchlorofluoride	132	CH3ClFPS	027127-27-1	27
2	1,4-Dithiacyclohept-2-ene	132	C5H8S2	070063-50-2	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





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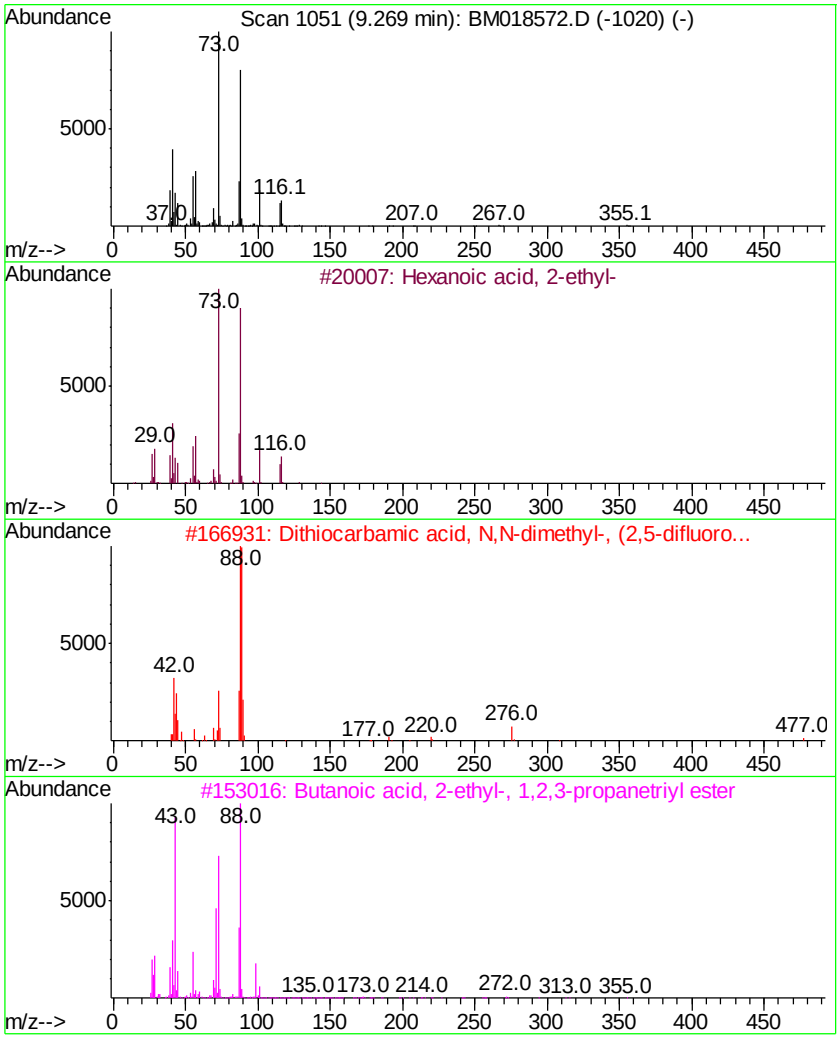
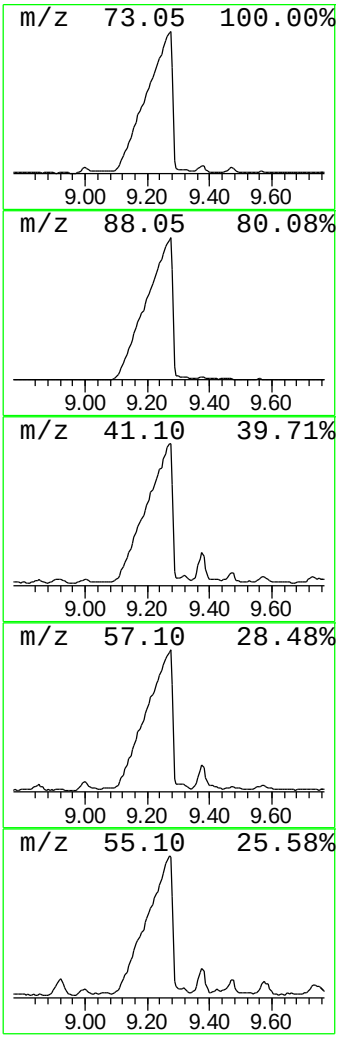
Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	213.24 ng	15935600	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Dithiocarbamic acid, N,N-dimethy...	477	C13H12F9N3S3	1000268-72-7	42
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
4	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
5	Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	38





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ClientSampleId : COMP-1

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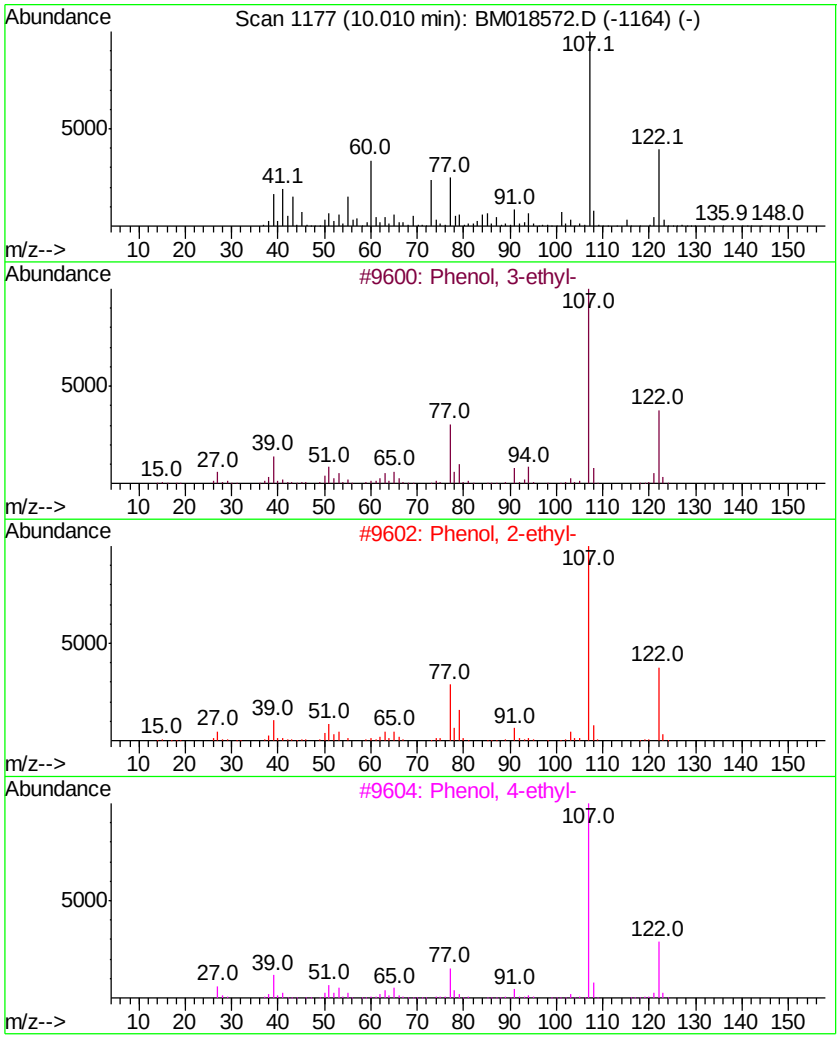
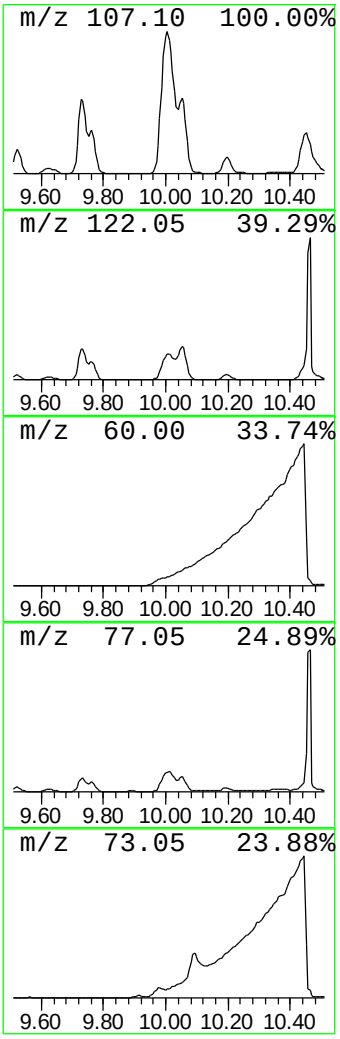
Peak Number 10 Phenol, 3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.01	101.21 ng	7563790	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	93
2	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	76
3	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	70
4	3,3-Dimethyl-6-methylenecyclohexene	122	C9H14	020185-16-4	53
5	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	40





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ClientSampleId : COMP-1

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TIC Library : C:\DATABASE\NIST02.L
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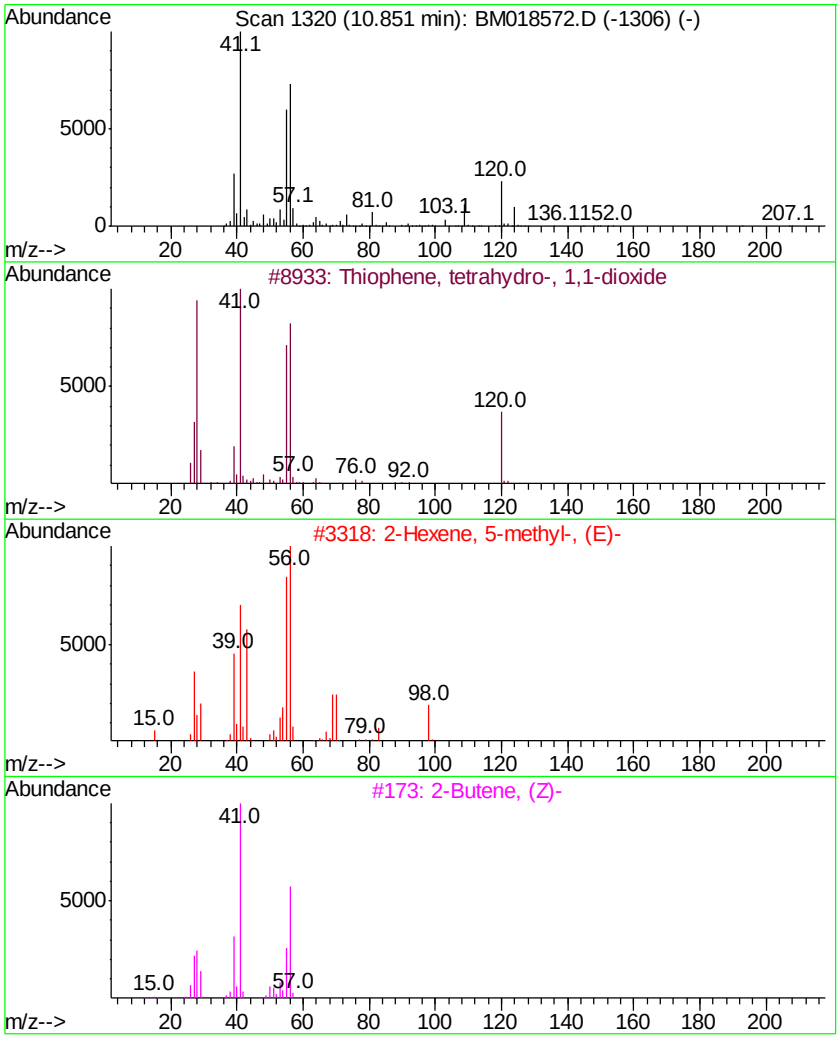
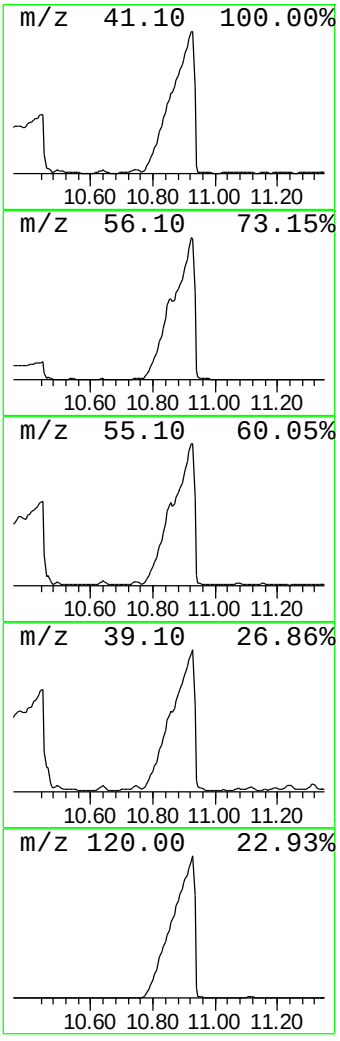
Peak Number 11 Thiophene, tetrahydro-, 1,1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	212.55 ng	15883800	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-, 1,1-dioxide	120	C4H8O2S	000126-33-0	76
2	2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	47
3	2-Butene, (Z)-	56	C4H8	000590-18-1	46
4	2-Butene, (E)-	56	C4H8	000624-64-6	43
5	Cyclobutane	56	C4H8	000287-23-0	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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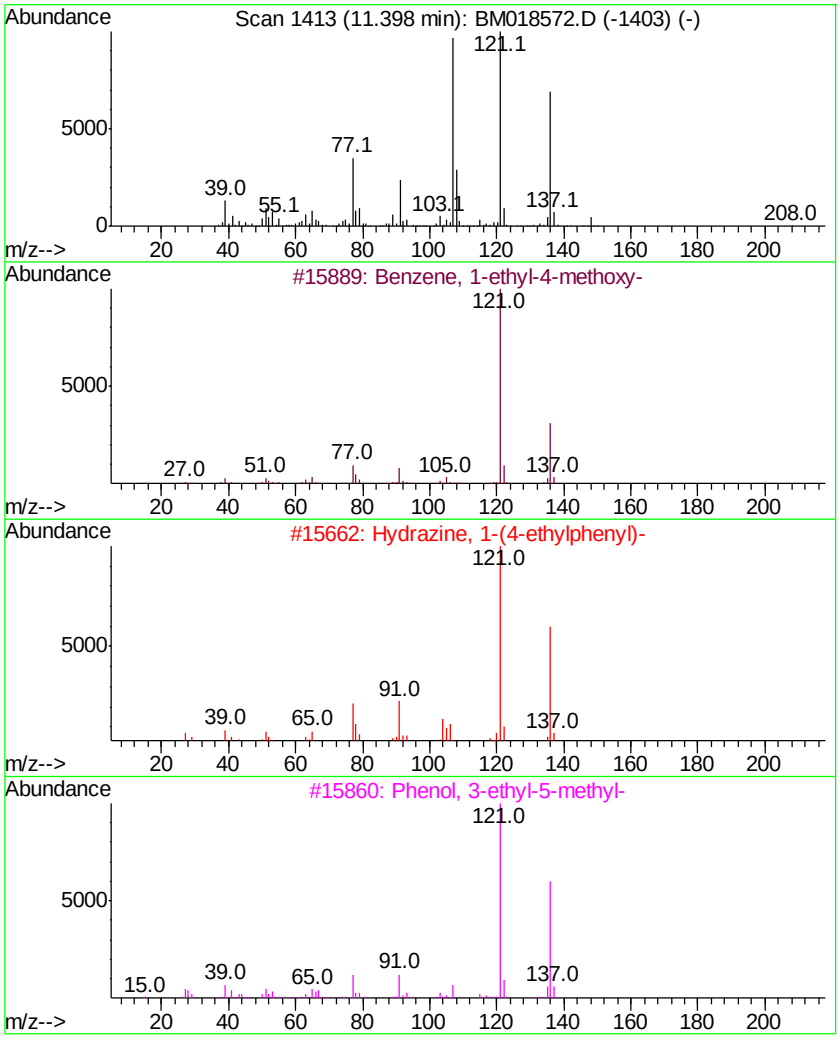
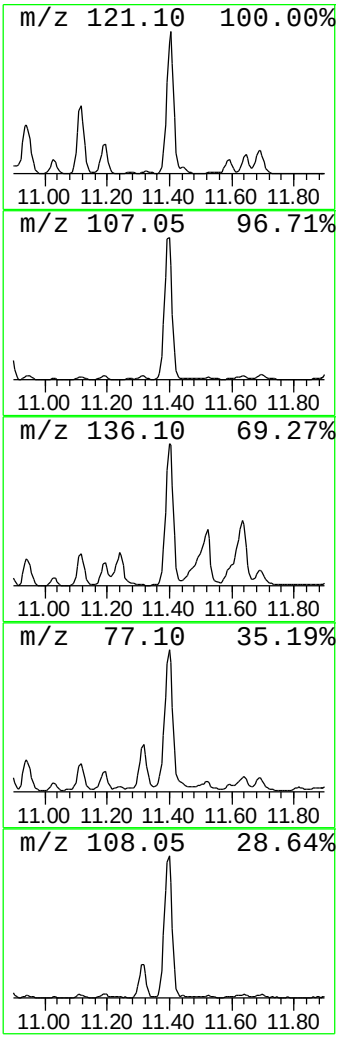
Peak Number 12 Benzene, 1-ethyl-4-methoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	103.80 ng	7756940	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	53
2	Hydrazine, 1-(4-ethylphenyl)-	136	C8H12N2	054840-34-5	49
3	Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	49
4	Phenol, 2,3,5-trimethyl-	136	C9H12O	000697-82-5	46
5	Phenol, 2,3,6-trimethyl-	136	C9H12O	002416-94-6	46





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Misc :
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Instrument : BNA_M
ClientSampleId : COMP-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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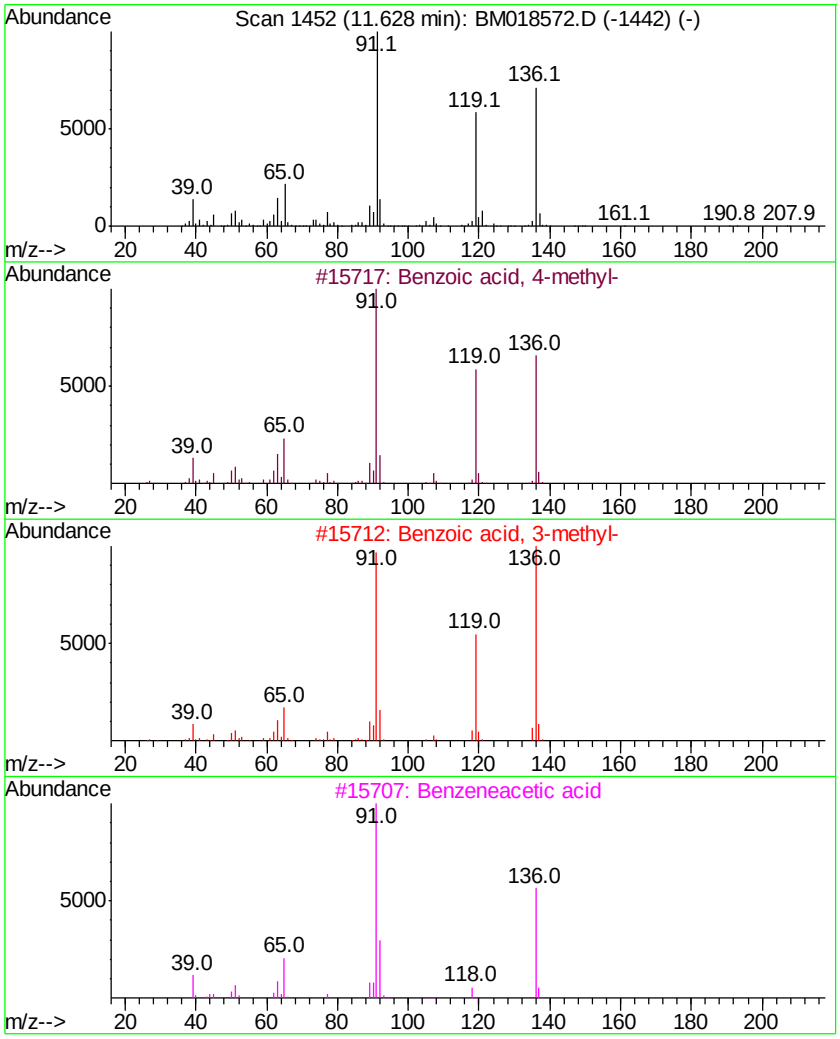
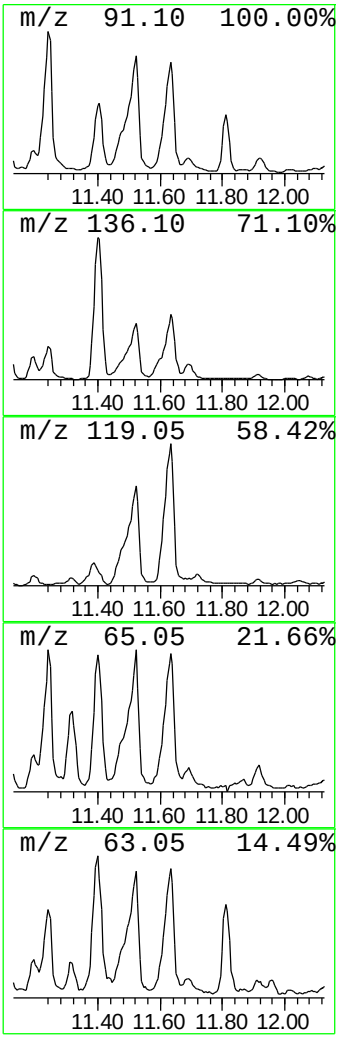
Peak Number 14 Benzoic acid, 4-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	37.80 ng	2824630	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	96
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	90
3	Benzeneacetic acid	136	C8H8O2	000103-82-2	64
4	Benzamide, 4-methyl-	135	C8H9NO	000619-55-6	41
5	3,5,7-Trimethyl-1,2(4H)-diazepine	136	C8H12N2	088829-73-6	38





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ClientSampleId : COMP-1

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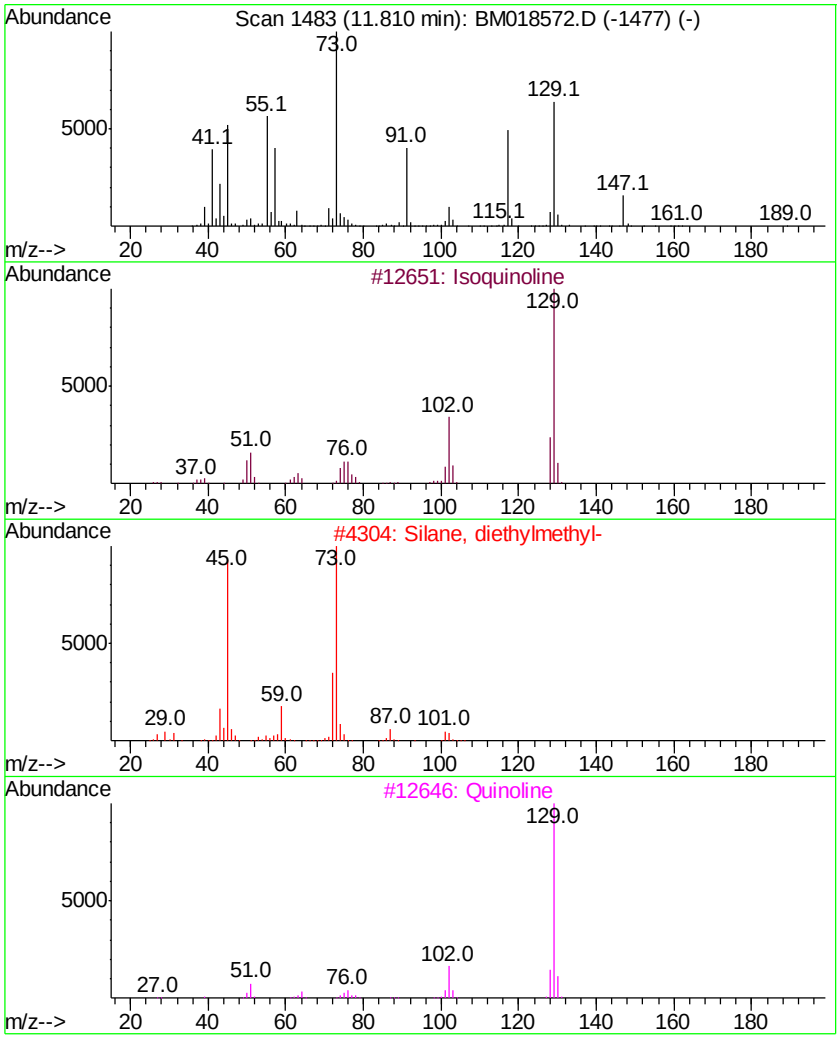
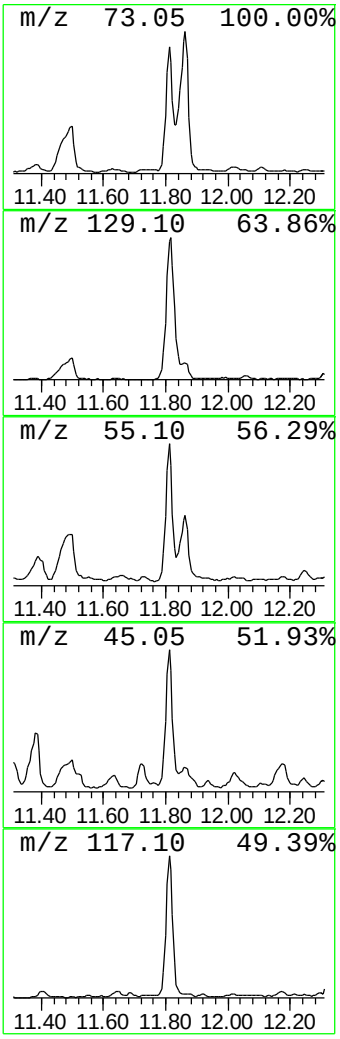
Peak Number 15 unknown11.81 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	46.00 ng	3437620	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoquinoline	129	C9H7N	000119-65-3	35
2	Silane, diethylmethyl-	102	C5H14Si	000760-32-7	22
3	Quinoline	129	C9H7N	000091-22-5	18
4	2-Methylbutane-1,4-diol, 3-(1-et...	192	C9H20O4	088481-54-3	14
5	1,3-Butanediol, 2-methyl-	104	C5H12O2	000684-84-4	10





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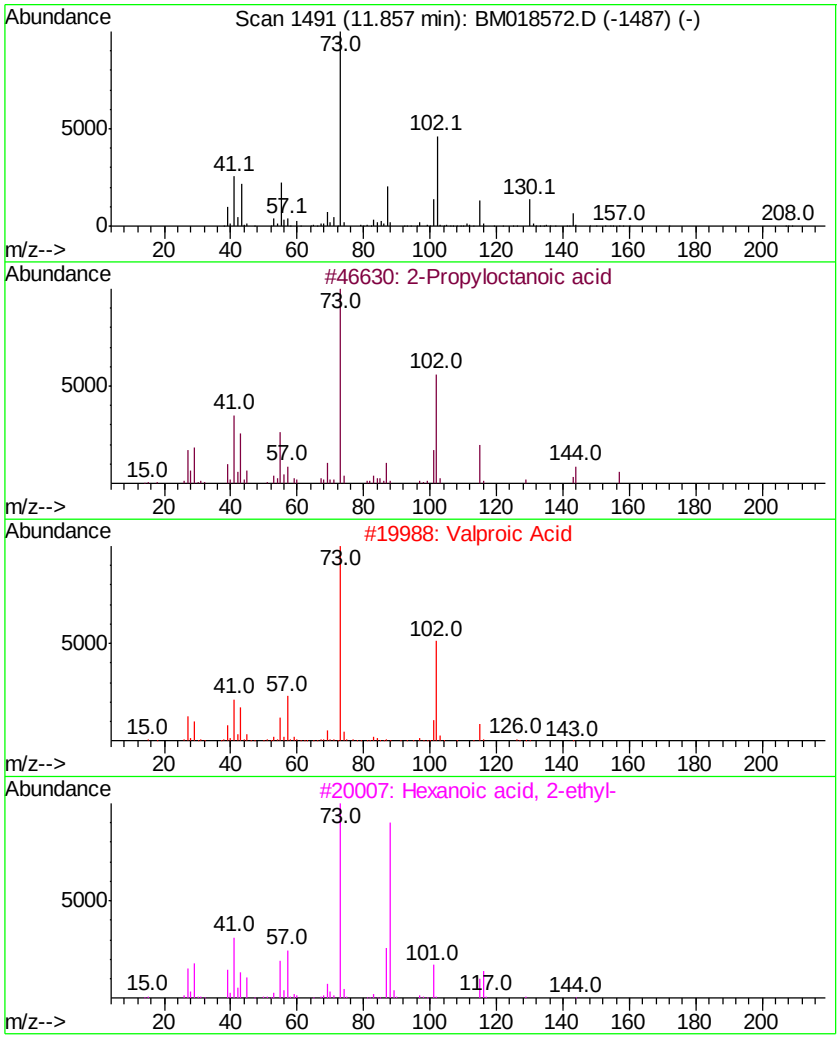
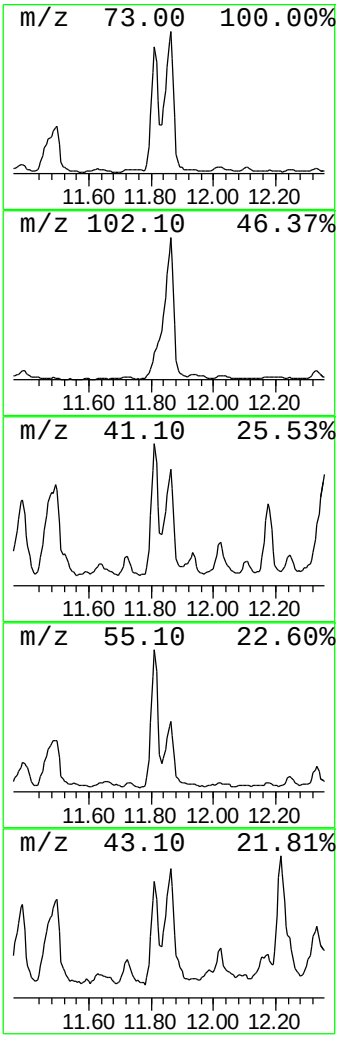
Peak Number 16 2-Propyloctanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	30.79 ng	2300900	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyloctanoic acid	186	C11H22O2	031080-41-8	53
2	Valproic Acid	144	C8H16O2	000099-66-1	40
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	35
4	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	10
5	Scyllo-Inositol, 1-C-methyl-	194	C7H14O6	000564-92-1	9





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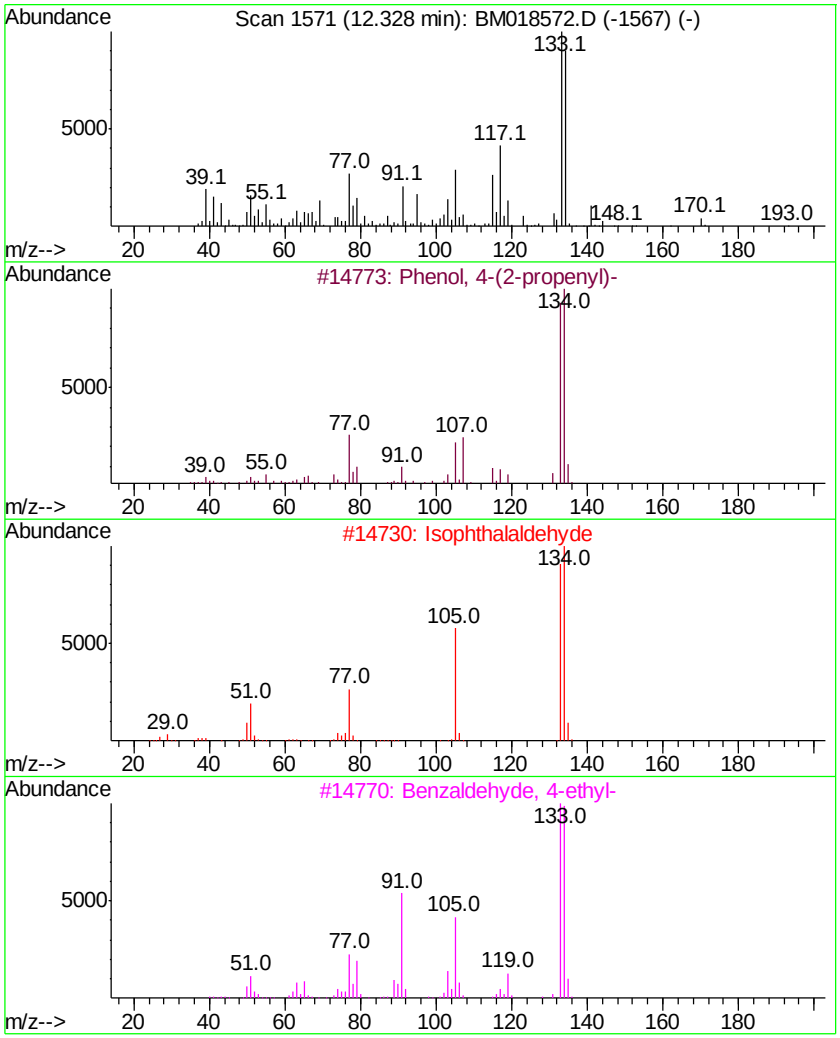
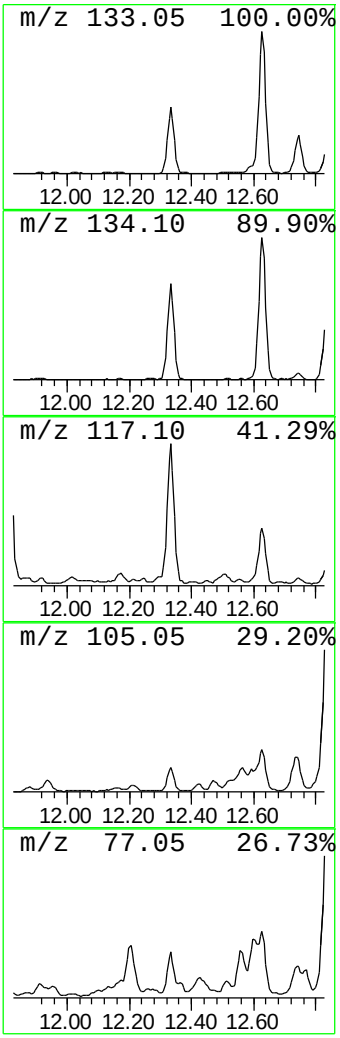
Peak Number 17 Phenol, 4-(2-propenyl)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	42.77 ng	3196320	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(2-propenyl)-	134	C9H10O	000501-92-8	58
2	Isophthalaldehyde	134	C8H6O2	000626-19-7	55
3	Benzaldehyde, 4-ethyl-	134	C9H10O	004748-78-1	53
4	Benzaldehyde, 2,4-dimethyl-	134	C9H10O	015764-16-6	53
5	2,6-Dimethylbenzaldehyde	134	C9H10O	001123-56-4	53





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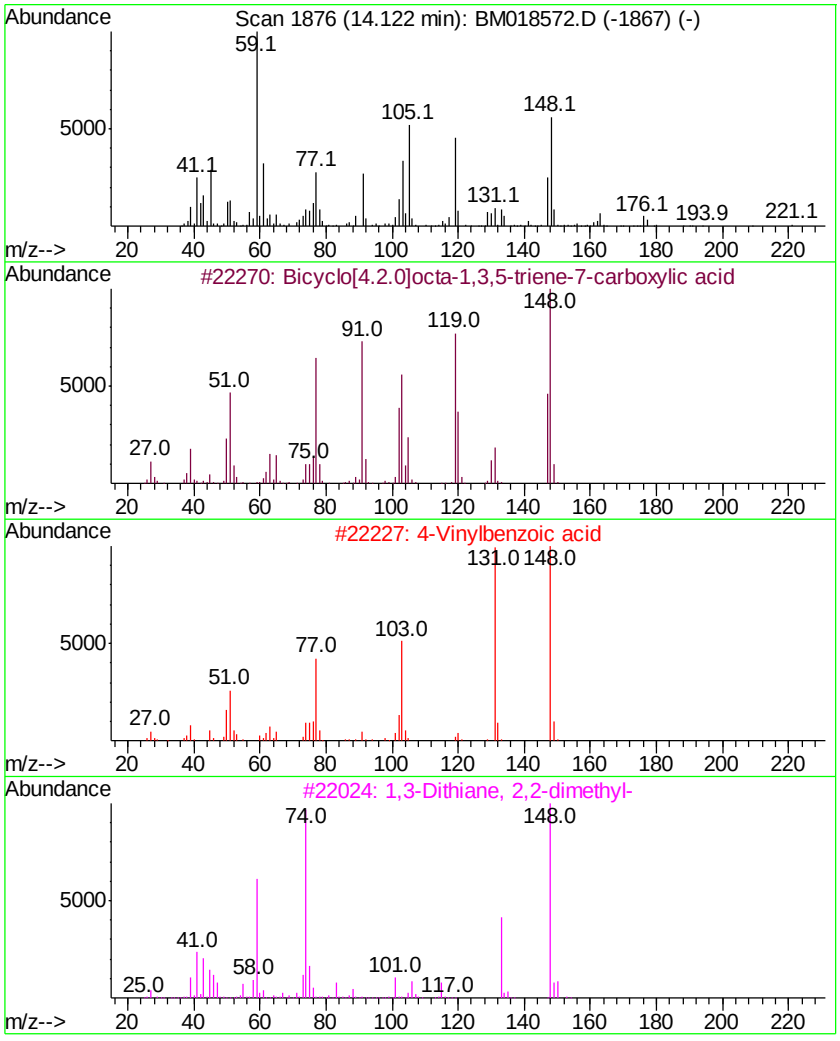
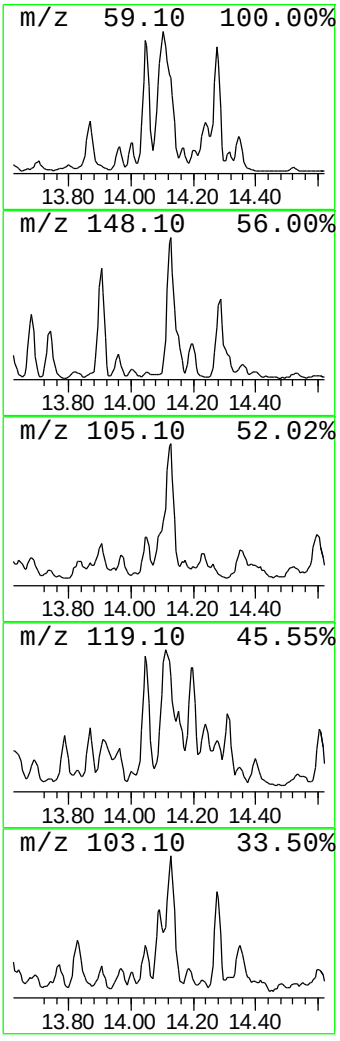
Peak Number 18 unknown14.12 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.12	30.83 ng	4191260	Acenaphthene-d10	14.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene-...	148	C9H8O2	014381-41-0	49
2	4-Vinylbenzoic acid	148	C9H8O2	001075-49-6	38
3	1,3-Dithiane, 2,2-dimethyl-	148	C6H12S2	006007-22-3	35
4	trans-Cinnamic acid	148	C9H8O2	000140-10-3	25
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	22





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Acq On : 15 Jan 2019 21:53
Operator : JU/SJ
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

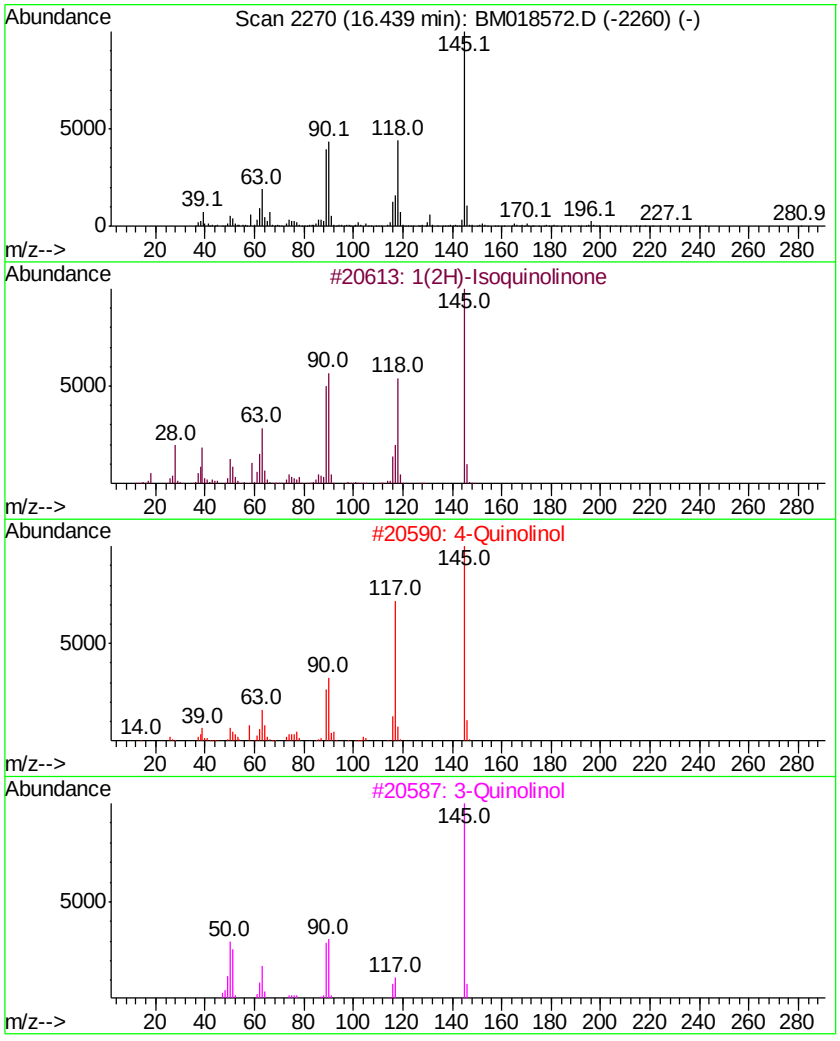
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

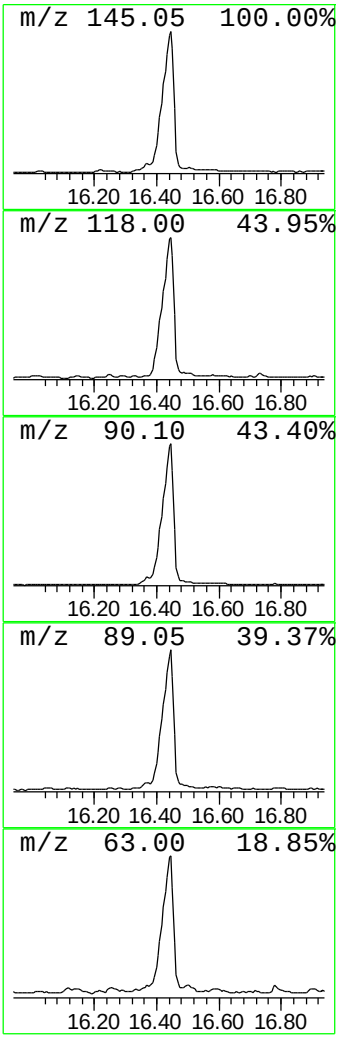
****

Peak Number 19 1(2H)-Isoquinolinone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	32.83 ng	5062320	Phenanthrene-d10	17.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Isoquinolinone	145	C9H7NO	000491-30-5	96
2	4-Quinolinol	145	C9H7NO	000611-36-9	81
3	3-Quinolinol	145	C9H7NO	000580-18-7	74
4	Isoquinoline, 2-oxide	145	C9H7NO	001532-72-5	72
5	2(1H)-Quinolinone	145	C9H7NO	000059-31-4	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
Data File : BM018572.D
Acq On : 15 Jan 2019 21:53
Operator : JU/SJ
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

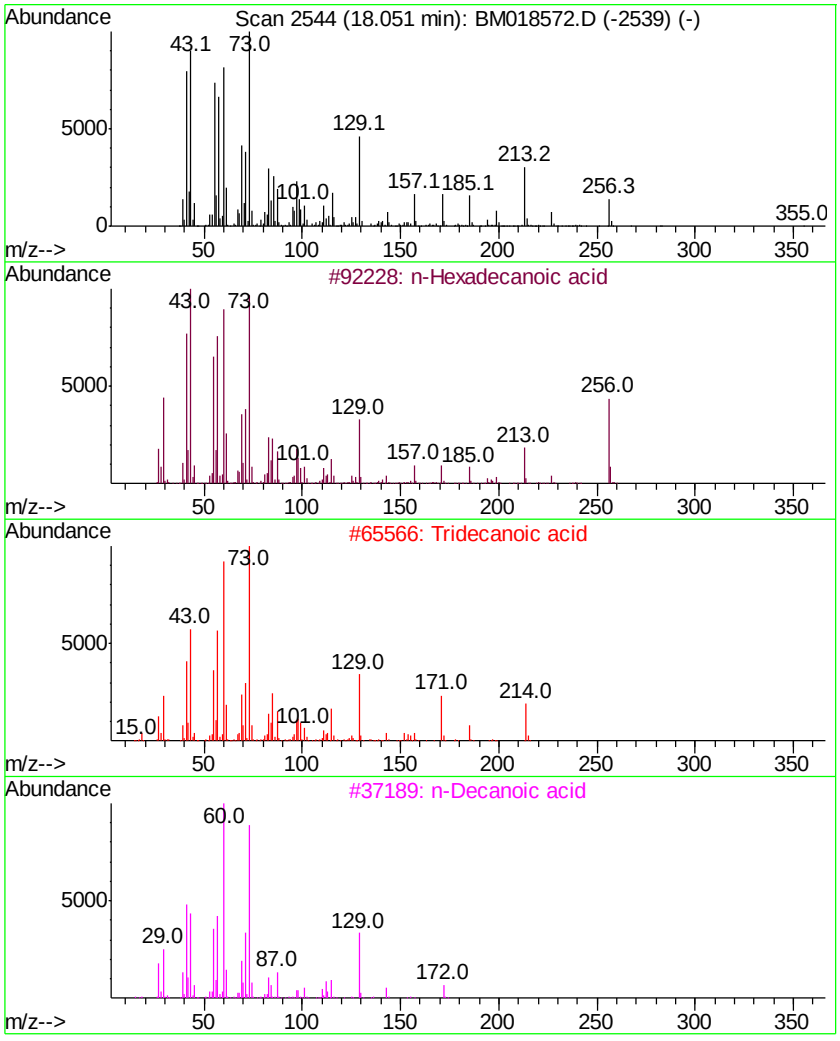
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

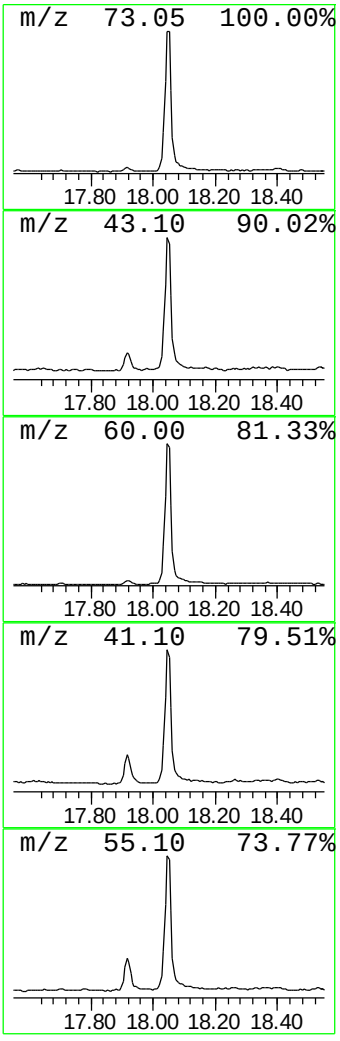
****

Peak Number 20 n-Hexadecanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	31.78 ng	4900200	Phenanthrene-d10	17.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011519\
Data File : BM018572.D
Acq On : 15 Jan 2019 21:53
Operator : JU/SJ
Sample : K1127-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Propanoic acid, 2...	3.63	39.1	ng	2241550	1	7.75	1145400	20.0
Butanoic acid	4.33	561.0	ng	32126500	1	7.75	1145400	20.0
unknown4.95	4.95	70.8	ng	4055180	1	7.75	1145400	20.0
Butanoic acid, 2-...	5.10	42.6	ng	2439040	1	7.75	1145400	20.0
Pentanoic acid	5.51	83.4	ng	4778130	1	7.75	1145400	20.0
Hexylene Glycol	6.16	80.8	ng	4624730	1	7.75	1145400	20.0
unknown7.29	7.29	64.9	ng	3716230	1	7.75	1145400	20.0
Hexanoic acid, 2-...	9.27	213.2	ng	15935600	2	10.55	1494630	20.0
Phenol, 3-ethyl-	10.01	101.2	ng	7563790	2	10.55	1494630	20.0
Thiophene, tetrah...	10.85	212.6	ng	15883800	2	10.55	1494630	20.0
Benzene, 1-ethyl-...	11.40	103.8	ng	7756940	2	10.55	1494630	20.0
Benzoic acid, 4-m...	11.63	37.8	ng	2824630	2	10.55	1494630	20.0
unknown11.81	11.81	46.0	ng	3437620	2	10.55	1494630	20.0
2-Propyloctanoic ...	11.86	30.8	ng	2300900	2	10.55	1494630	20.0
Phenol, 4-(2-prop...	12.33	42.8	ng	3196320	2	10.55	1494630	20.0
unknown14.12	14.12	30.8	ng	4191260	3	14.40	2719390	20.0
1(2H)-Isoquinolinone	16.44	32.8	ng	5062320	4	17.15	3084310	20.0
n-Hexadecanoic acid	18.05	31.8	ng	4900200	4	17.15	3084310	20.0