LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099021.D
Acq On : 3 Oct 2017 1:10
Operator : SJ/JU
Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.181	13	16	27	rVB	53077	96054	12.75%	0.907%
2	4.510	408	412	417	rBV	97041	101852	13.52%	0.961%
3	5.122	511	516	524	rBV	693186	710968	94.34%	6.711%
4	5.516	580	583	590	rVB	203196	166331	22.07%	1.570%
5	6.522	750	754	762	rBV	651726	551390	73.17%	5.205%
6	6.669	776	779	783	rVB	416817	328128	43.54%	3.097%
7	6.904	815	819	823	rVB	833954	656572	87.13%	6.198%
8	6.957	824	828	831	rBV	40643	33525	4.45%	0.316%
9	7.057	840	845	849	rBV	652326	546479	72.52%	5.158%
10	7.433	902	909	910	rBV2	10193	14087	1.87%	0.133%
11	7.463	910	914	917	rVV	434850	367729	48.80%	3.471%
12	7.492	917	919	923	rVV2	13496	14394	1.91%	0.136%
13	7.539	923	927	931	rVB4	10624	15447	2.05%	0.146%
14	7.598	931	937	940	rBV3	5388	9588	1.27%	0.091%
15	7.710	952	956	958	rVB3	8955	10107	1.34%	0.095%
16	7.922	989	992	995	rBV3	10662	12068	1.60%	0.114%
17	8.051	1011	1014	1017	rBV4	8545	9787	1.30%	0.092%
18	8.186	1033	1037	1040	rBV	949613	753588	100.00%	7.113%
19	8.233	1043	1045	1048	rVB	41759	40168	5.33%	0.379%
20	8.269	1048	1051	1056	rVB5	12318	17036	2.26%	0.161%
21	8.386	1068	1071	1074	rVB2	12031	10579	1.40%	0.100%
22	8.469	1082	1085	1090	rVB5	21495	29201	3.87%	0.276%
23	8.527	1090	1095	1097	rBV3	8725	12479	1.66%	0.118%
24	8.569	1098	1102	1104	rVB5	9135	10231	1.36%	0.097%
25	8.598	1104	1107	1109	rBV	48870	38818	5.15%	0.366%
26	8.645	1113	1115	1119	rVB4	12121	12024	1.60%	0.113%
27	8.686	1119	1122	1124	rBV2	17696	14848	1.97%	0.140%
28	8.722	1124	1128	1130	rBV4	11712	12435	1.65%	0.117%
29	8.769	1134	1136	1140	rVV3	23063	20664	2.74%	0.195%
30	8.804	1140	1142	1145	rVV4	10311	13747	1.82%	0.130%
31	8.863	1149	1152	1156	rVB3	19293	29057	3.86%	0.274%
32	8.898	1156	1158	1160	rBV2	12375	10186	1.35%	0.096%
33	8.933	1161	1164	1166	rVB3	12313	10321	1.37%	0.097%
34	8.957	1166	1168	1171	rBV4	11829	13935	1.85%	0.132%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.004	1171	1176	1178	rVV2	19236	24802	3.29%	0.234%
36	9.063	1182	1186	1188	rBV4	11454	18090	2.40%	0.171%
37	9.086	1188	1190	1194	rVB4	17302	19190	2.55%	0.181%
38	9.127	1194	1197	1203	rBV6	13168	21120	2.80%	0.199%
39	9.175	1203	1205	1207	rBV	10438	10215	1.36%	0.096%
40	9.198	1207	1209	1215	rVB	65118	50444	6.69%	0.476%
41	9.257	1215	1219	1224	rBV	818483	653774	86.75%	6.171%
42	9.333	1229	1232	1236	rBV2	43121	53758	7.13%	0.507%
43	9.410	1243	1245	1248	rVB4	17266	14254	1.89%	0.135%
44	9.527	1261	1265	1268	rBV3	28367	41356	5.49%	0.390%
45	9.598	1274	1277	1280	rBV	34043	40007	5.31%	0.378%
46	9.627	1280	1282	1283	rVV	19755	14113	1.87%	0.133%
47	9.651	1283	1286	1290	rVV	191099	167455	22.22%	1.581%
48	9.716	1293	1297	1299	rBV4	23227	23131	3.07%	0.218%
49	9.804	1309	1312	1315	rBV3	37112	33208	4.41%	0.313%
50	9.851	1318	1320	1325	rVV2	35546	48055	6.38%	0.454%
51	9.898	1326	1328	1330	rVV3	13291	16562	2.20%	0.156%
52	9.945	1330	1336	1339	rVV	793128	722664	95.90%	6.821%
53	9.974	1339	1341	1345	rVV4	26470	32067	4.26%	0.303%
54	10.045	1349	1353	1357	rBV3	21580	33162	4.40%	0.313%
55	10.086	1357	1360	1364	rBV5	9792	13072	1.73%	0.123%
56	10.121	1364	1366	1367	rBV2	14029	10813	1.43%	0.102%
57	10.139	1367	1369	1374	rVB2	31106	33400	4.43%	0.315%
58	10.186	1374	1377	1386	rVB3	41593	61633	8.18%	0.582%
59	10.257	1386	1389	1391	rBV	35072	32388	4.30%	0.306%
60	10.286	1391	1394	1396	rVB3	17915	13349	1.77%	0.126%
61	10.345	1401	1404	1406	rBV3	31534	43787	5.81%	0.413%
62	10.363	1406	1407	1409	rVB2	38170	20738	2.75%	0.196%
63	10.392	1409	1412	1415	rBV4	12115	12046	1.60%	0.114%
64	10.416	1415	1416	1422	rVB6	10443	18614	2.47%	0.176%
65	10.486	1422	1428	1430	rBV4	17973	28466	3.78%	0.269%
66	10.580	1441	1444	1450	rVB	69519	78153	10.37%	0.738%
67	10.639	1450	1454	1455	rBV4	11006	12130	1.61%	0.114%
68	10.704	1463	1465	1467	rVB2	14542	11336	1.50%	0.107%
69	10.727	1467	1469	1473	rBV5	12697	17073	2.27%	0.161%
70	10.851	1484	1490	1493	rBV	119860	150272	19.94%	1.418%
71	10.927	1501	1503	1506	rBV3	17496	16025	2.13%	0.151%

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

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
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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72	11.027	1518	1520	1522	rBV3	10818	11701	1.55%	0.110%
73	11.068	1524	1527	1530	rVB4	20937	23232	3.08%	0.219%
74	11.233	1553	1555	1558	rBV4	11943	12541	1.66%	0.118%
75	11.280	1560	1563	1566	rBV	56795	52863	7.01%	0.499%
76	11.316	1566	1569	1571	rVV	50838	46846	6.22%	0.442%
77	11.433	1585	1589	1591	rBV	720781	643994	85.46%	6.079%
78	11.451	1591	1592	1596	rVB	42099	34969	4.64%	0.330%
79	11.539	1604	1607	1610	rBV4	7627	11832	1.57%	0.112%
80	11.663	1626	1628	1634	rBV6	21918	22643	3.00%	0.214%
81	11.710	1634	1636	1639	rVB2	21745	17868	2.37%	0.169%
82	11.739	1639	1641	1650	rBV3	15733	33707	4.47%	0.318%
83	11.933	1671	1674	1677	rBV3	13573	17019	2.26%	0.161%
84	11.980	1680	1682	1684	rVB	21361	14828	1.97%	0.140%
85	12.039	1690	1692	1699	rVB6	17556	24307	3.23%	0.229%
86	12.115	1703	1705	1708	rBV2	15961	13607	1.81%	0.128%
87	12.339	1740	1743	1744	rBV3	13483	11599	1.54%	0.109%
88	12.404	1751	1754	1757	rBV4	11479	16096	2.14%	0.152%
89	12.439	1759	1760	1764	rVV4	10451	12695	1.68%	0.120%
90	12.504	1769	1771	1774	rBV2	15740	13590	1.80%	0.128%
91	12.610	1786	1789	1792	rVB4	10186	13960	1.85%	0.132%
92	12.645	1792	1795	1800	rBV	60088	60716	8.06%	0.573%
93	12.821	1823	1825	1828	rBV4	10567	11463	1.52%	0.108%
94	12.892	1831	1837	1841	rVV2	102513	161889	21.48%	1.528%
95	12.986	1851	1853	1854	rBV2	12650	9941	1.32%	0.094%
96	13.010	1854	1857	1861	rVV	668703	558939	74.17%	5.276%
97	13.086	1867	1870	1871	rBV3	12132	11609	1.54%	0.110%
98	13.486	1935	1938	1944	rBV	120485	104583	13.88%	0.987%
99	14.074	2034	2038	2041	rBV	760011	694866	92.21%	6.559%
100	15.568	2287	2292	2300	rVB	470762	625524	83.01%	5.905%

Sum of corrected areas: 10593972

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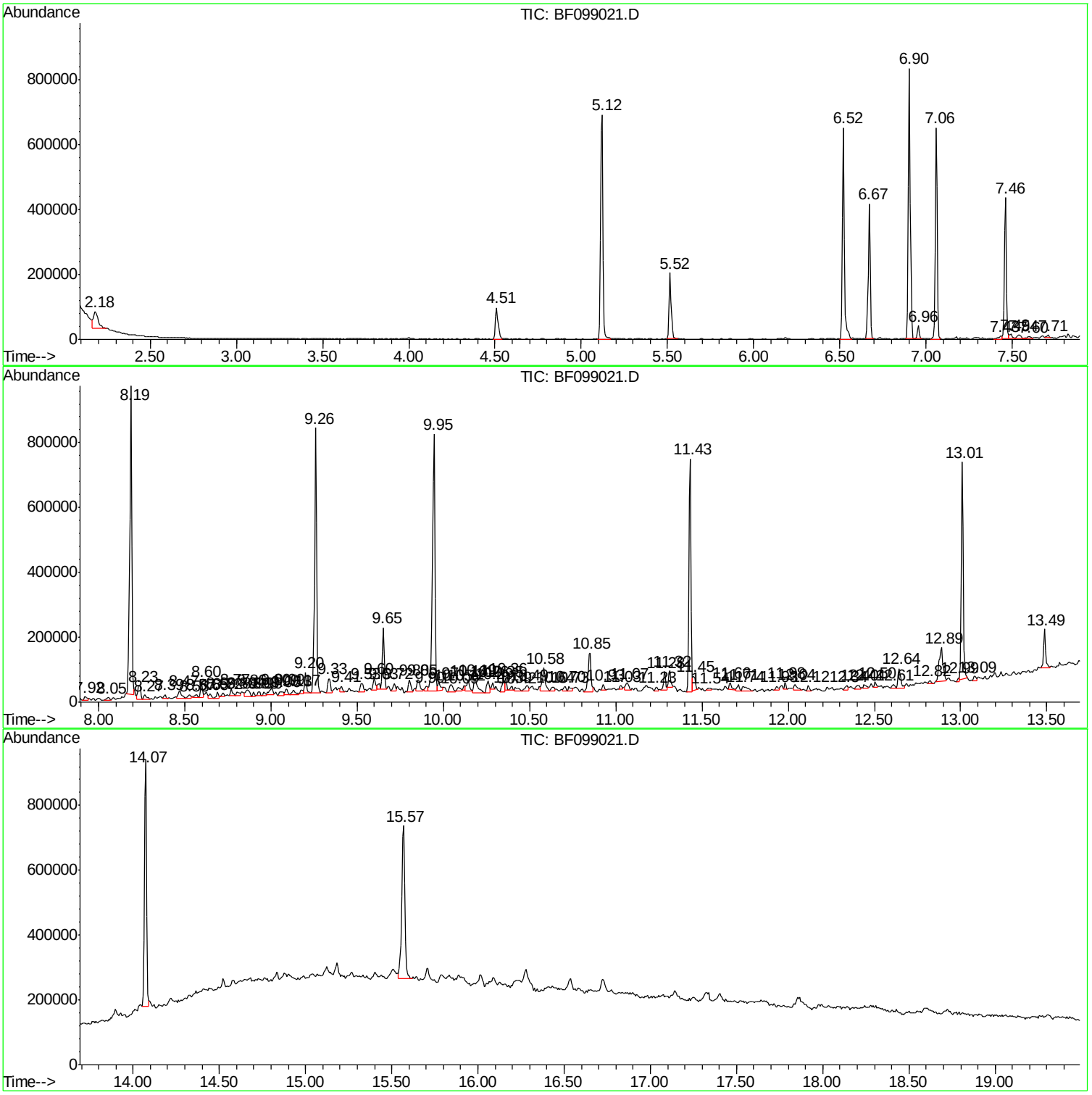
Operator : SJ/JU
Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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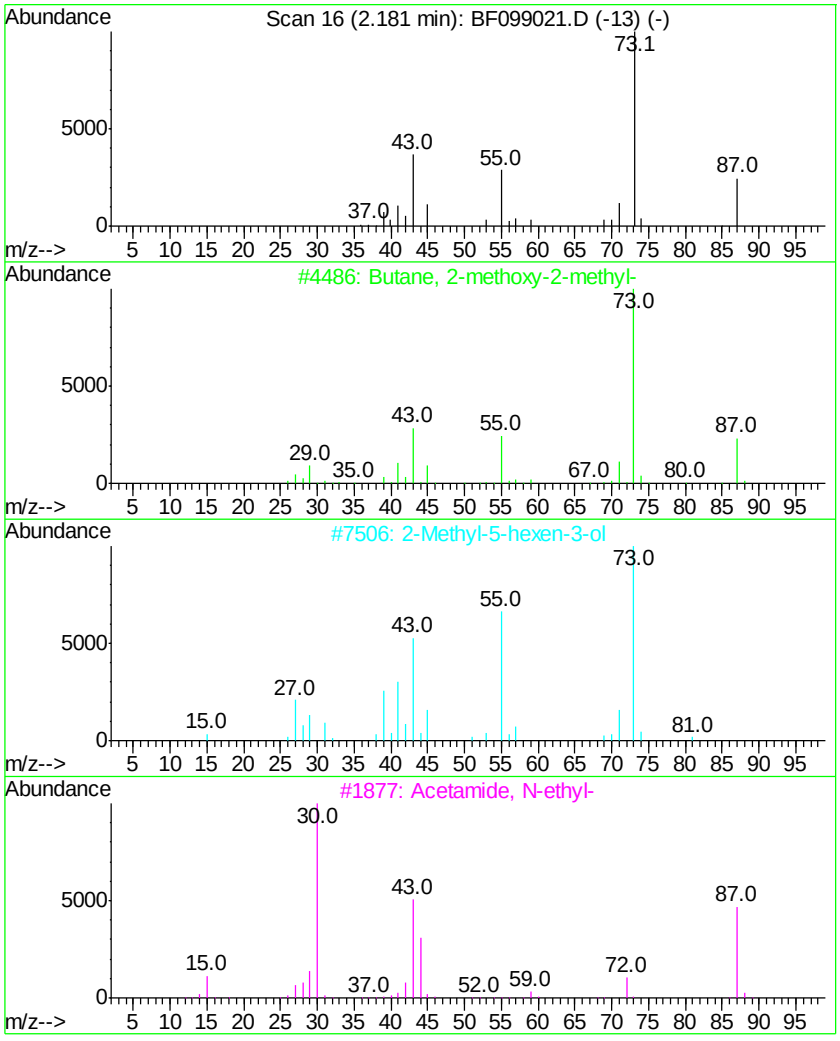
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

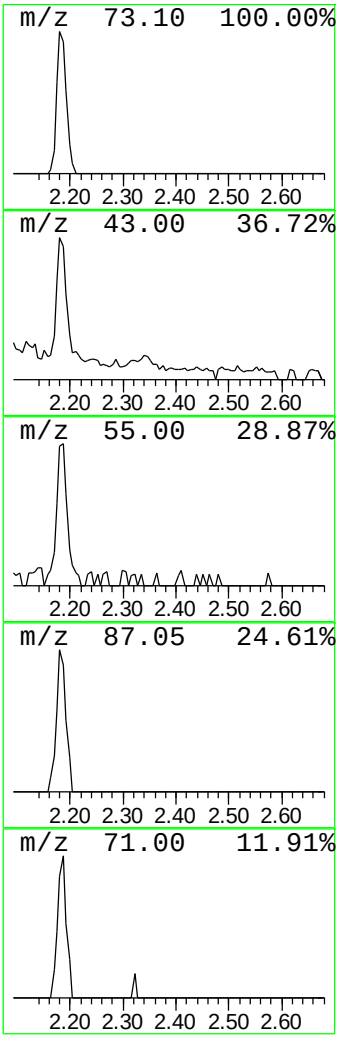
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	2.93 ng	96054	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	53
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





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Acq On : 3 Oct 2017 1:10
Operator : SJ/JU
Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

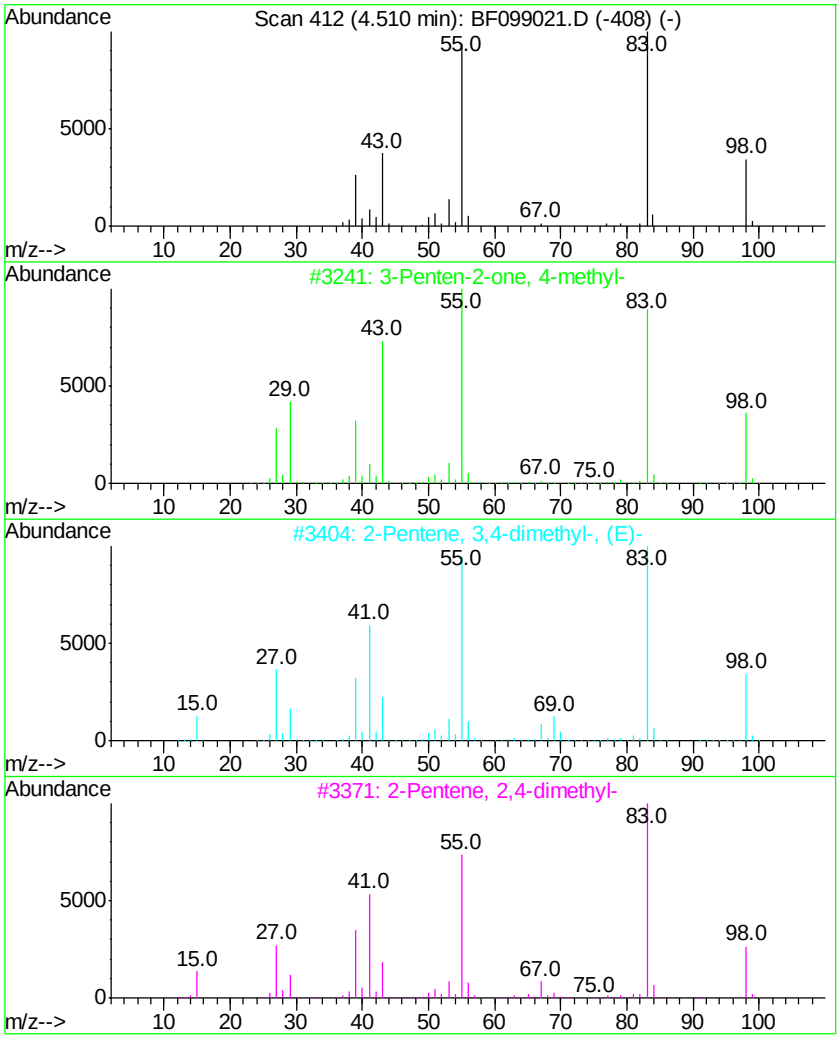
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

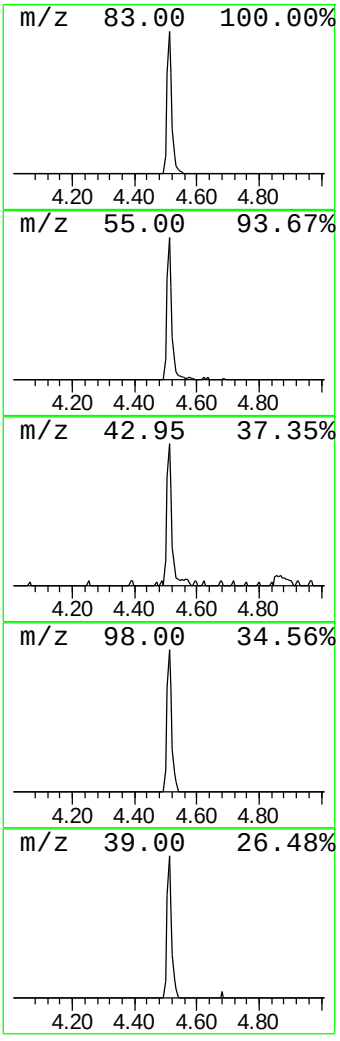
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.51	3.10 ng	101852	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4	3-Hexen-2-one	98	C6H10O	000763-93-9	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

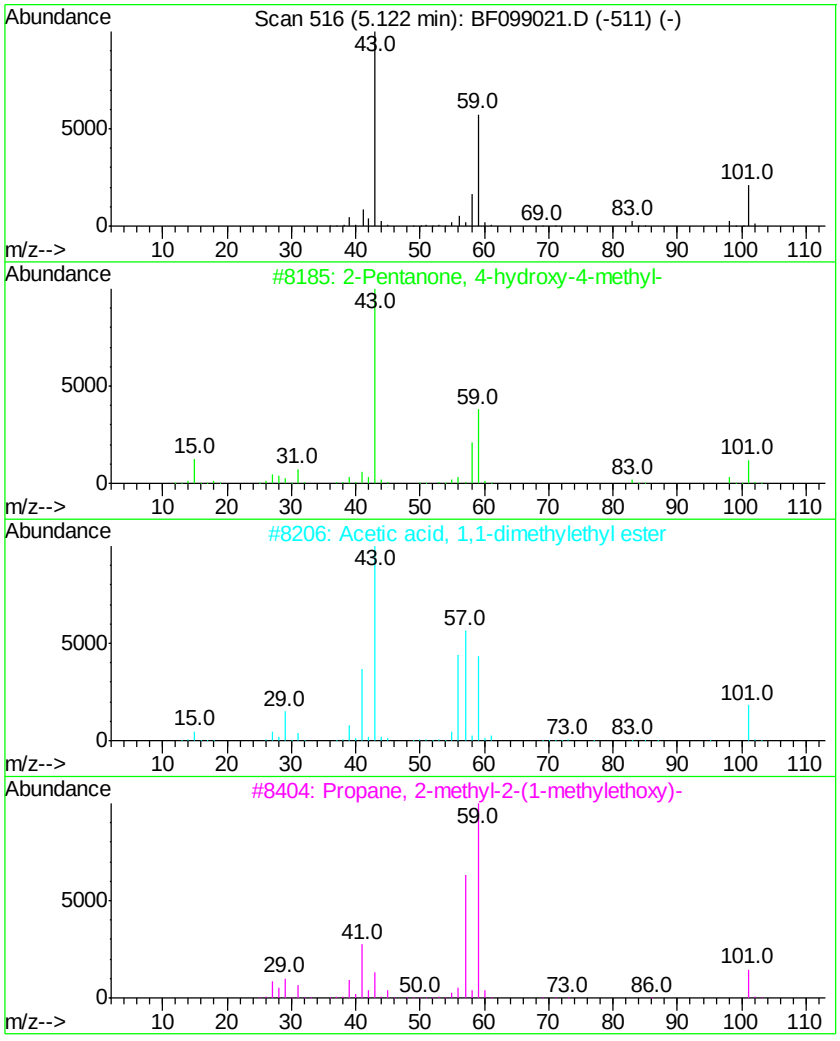
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

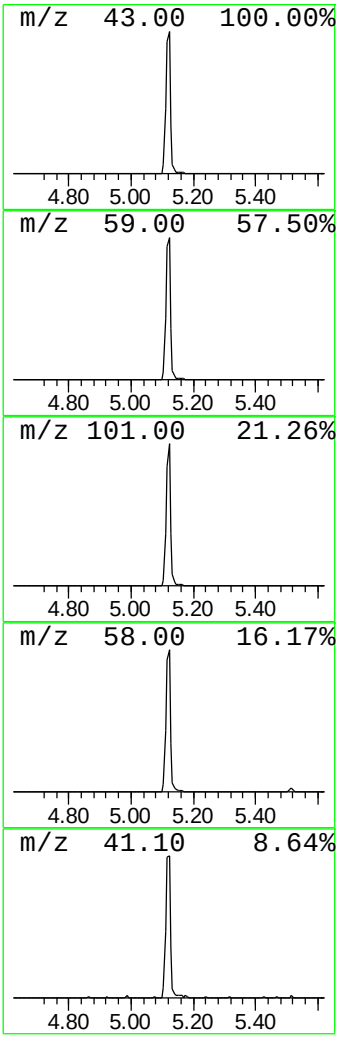
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	21.66 ng	710968	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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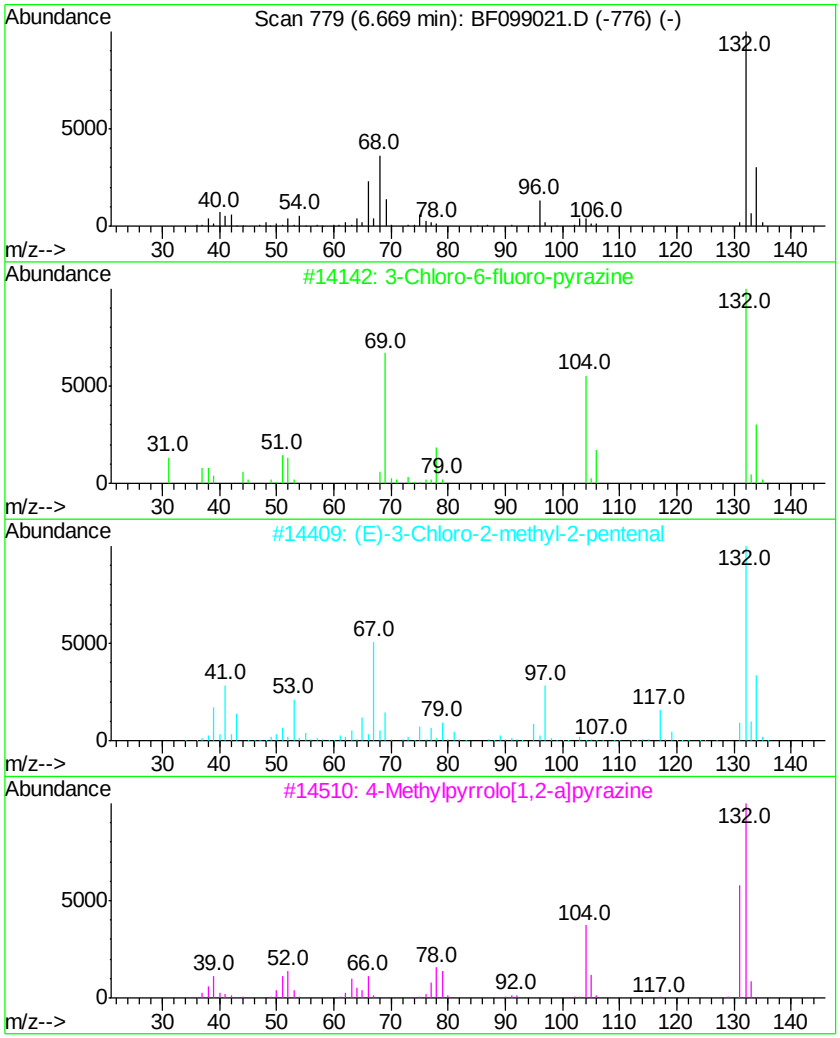
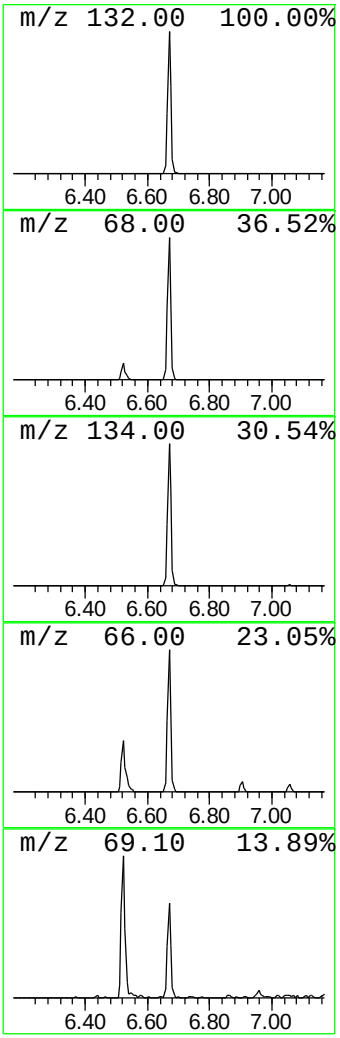
****

Peak Number 4 unknown6.67 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	10.00 ng	328128	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

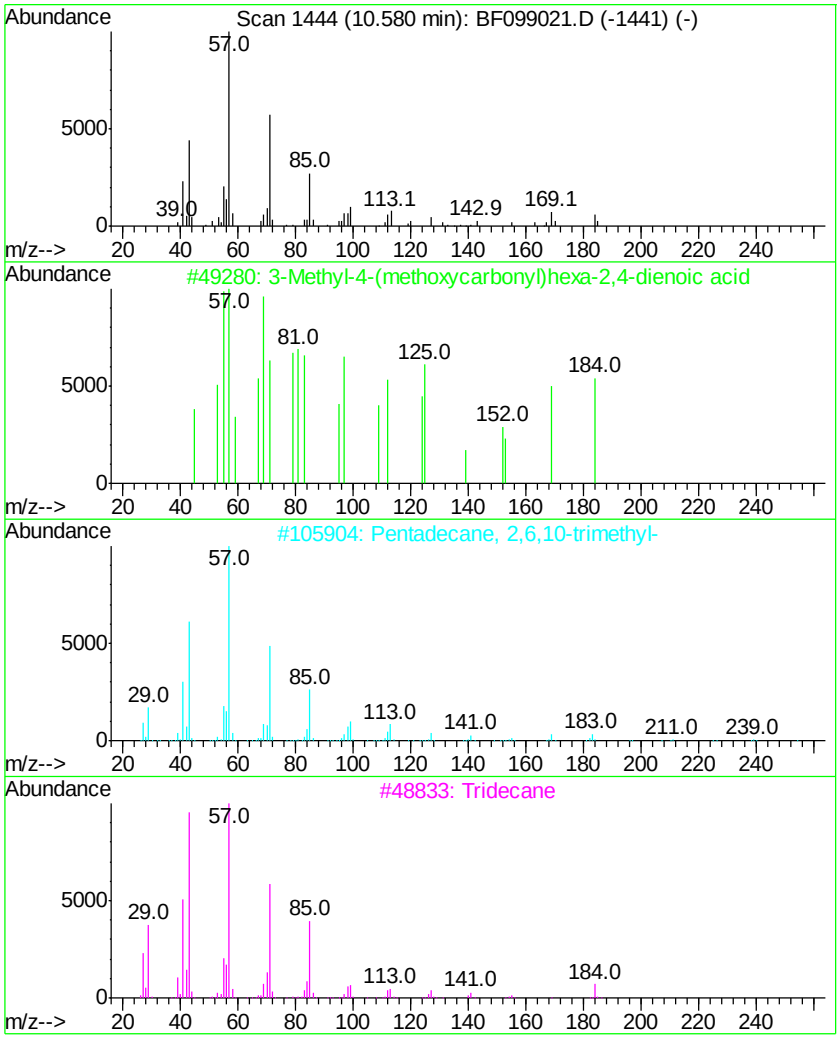
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

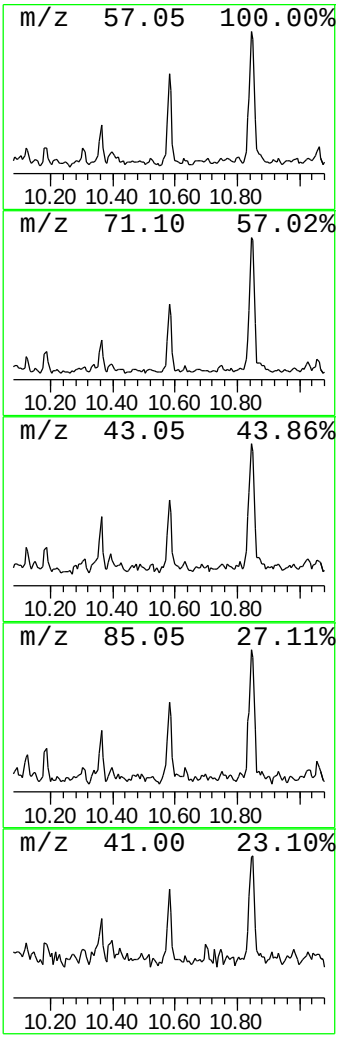
****

Peak Number 6 3-Methyl-4-(methoxycarbonyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	2.16 ng	78153	Acenaphthene-d10	9.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	92
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3	Tridecane	184	C13H28	000629-50-5	80
4	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	64
5	Triacontane	422	C30H62	000638-68-6	64





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Acq On : 3 Oct 2017 1:10
Operator : SJ/JU
Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

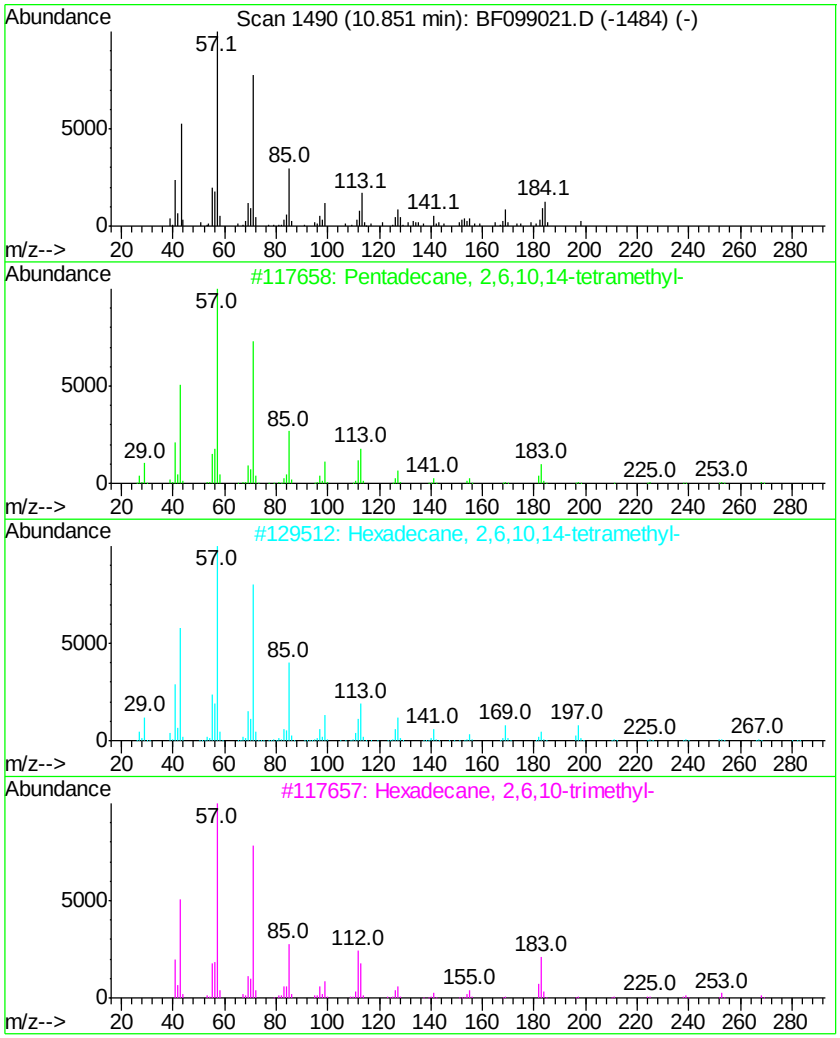
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

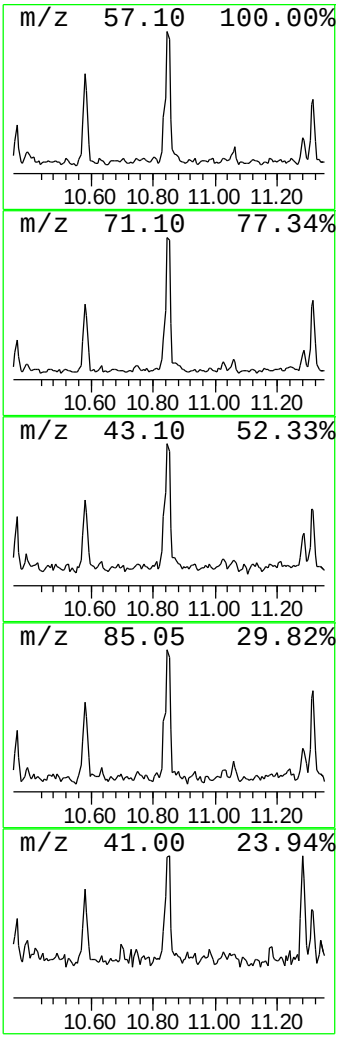
****

Peak Number 7 Pentadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	4.67 ng	150272	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	87
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	87
3	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	86
4	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	86
5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	68





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Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

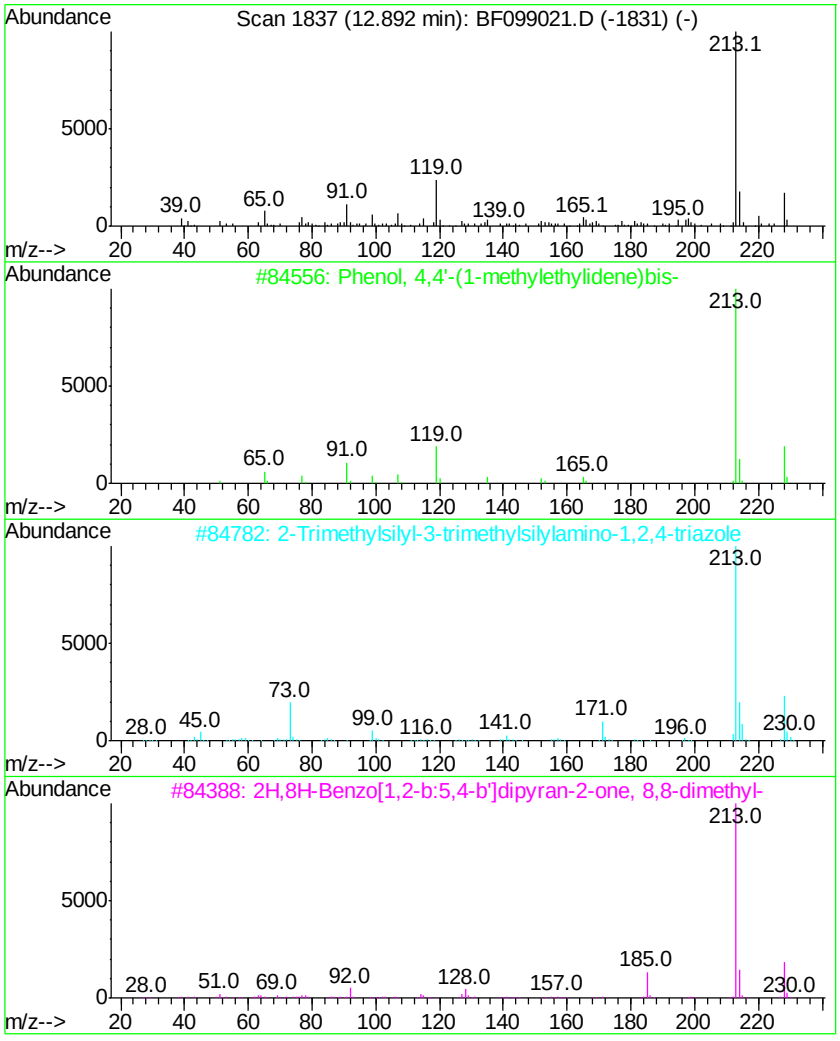
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

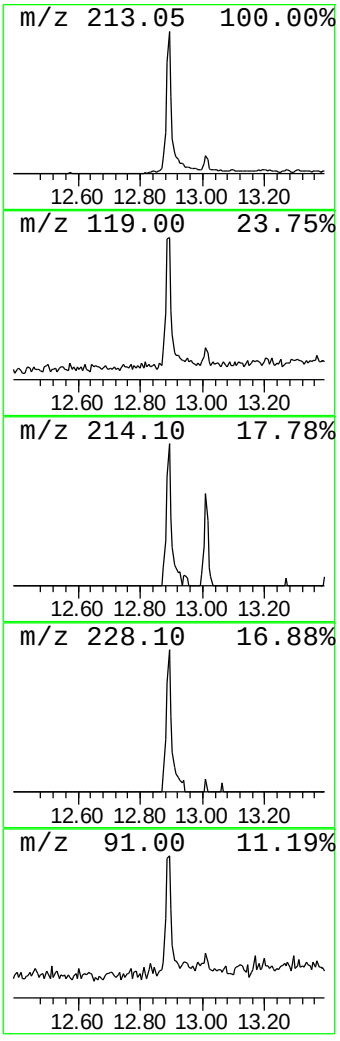
****

Peak Number 8 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	4.66 ng	161889	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	58
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	58
5	1,4-Naphthalenedione, 2-(1-buten...	228	C14H12O3	029366-43-6	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099021.D
Acq On : 3 Oct 2017 1:10
Operator : SJ/JU
Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

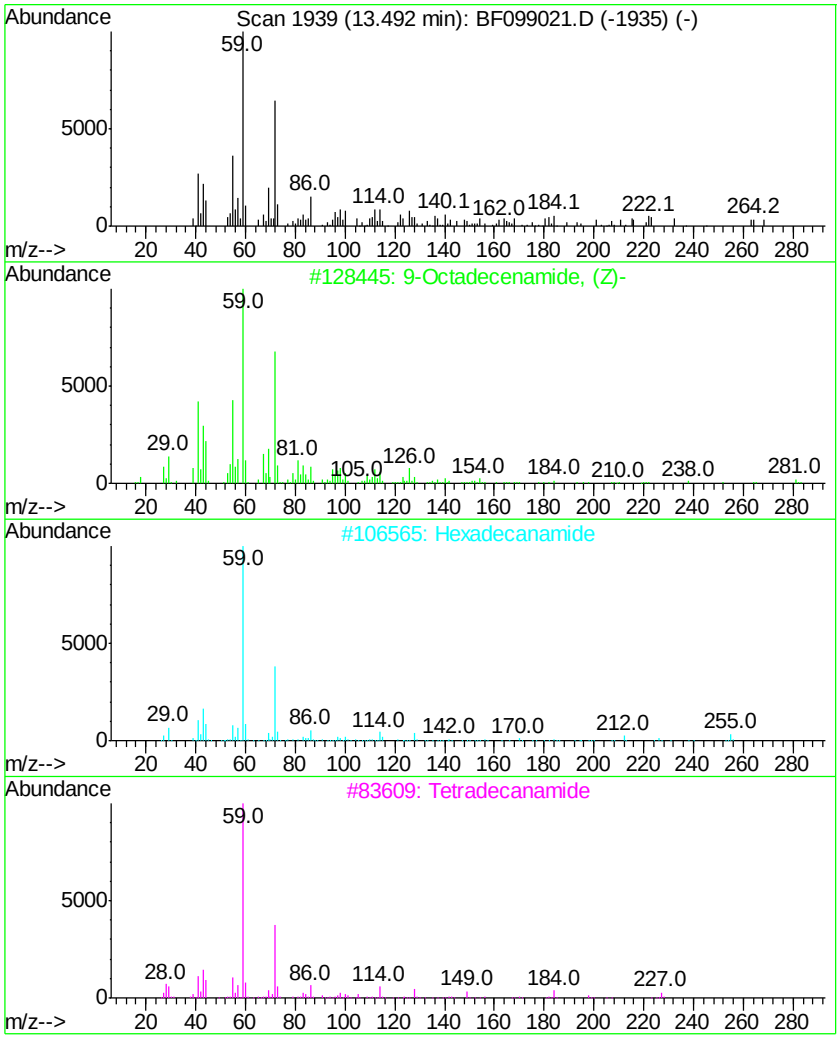
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

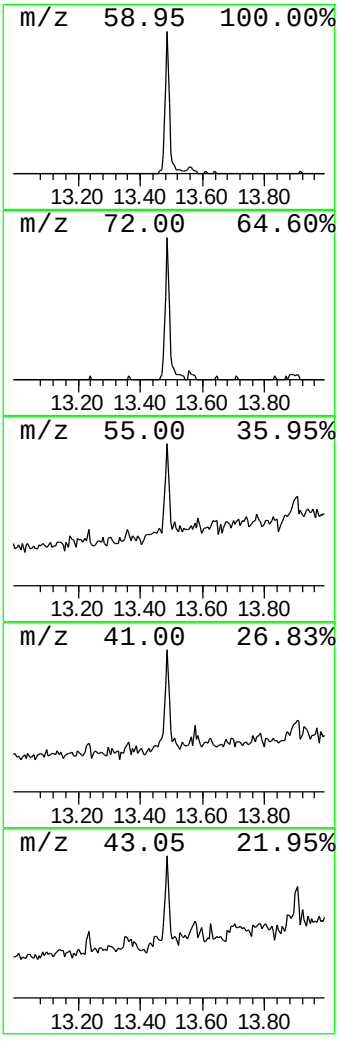
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.01 ng	104583	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Decanamide-	171	C10H21NO	002319-29-1	64
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
Data File : BF099021.D
Acq On : 3 Oct 2017 1:10
Operator : SJ/JU
Sample : I5531-05 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-63-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Butane, 2-methoxy...	2.18	2.9	ng	96054	1	6.90	656572	20.0
3-Penten-2-one, 4...	4.51	3.1	ng	101852	1	6.90	656572	20.0
2-Pentanone, 4-hy...	5.12	21.7	ng	710968	1	6.90	656572	20.0
unknown6.67	6.67	10.0	ng	328128	1	6.90	656572	20.0
3-Methyl-4-(metho...	10.58	2.2	ng	78153	3	9.95	722664	20.0
Pentadecane, 2,6,...	10.85	4.7	ng	150272	4	11.43	643994	20.0
Phenol, 4,4'-(1-m...	12.89	4.7	ng	161889	5	14.07	694866	20.0
9-Octadecenamide,...	13.49	3.0	ng	104583	5	14.07	694866	20.0