LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040815\
Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-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:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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	1.081	15	17	20	rBV	910621	984925	100.00%	6.534%
2	1.195	23	27	30	rVB	199926	304166	30.88%	2.018%
3	1.344	38	40	43	rVB	74245	82532	8.38%	0.548%
4	1.550	56	58	62	rBV	13854	22652	2.30%	0.150%
5	1.653	65	67	78	rBV	143639	219993	22.34%	1.459%
6	4.613	324	326	333	rVB	42208	74910	7.61%	0.497%
7	5.196	374	377	390	rVB	375730	601571	61.08%	3.991%
8	6.522	490	493	500	rBV	398855	629132	63.88%	4.174%
9	6.636	500	503	505	rBV	451191	637767	64.75%	4.231%
10	6.910	525	527	530	rVB	274803	253927	25.78%	1.685%
11	7.093	541	543	546	rBV	429224	455023	46.20%	3.019%
12	7.608	586	588	591	rBV	338447	364499	37.01%	2.418%
13	8.488	663	665	668	rBV	393972	348897	35.42%	2.315%
14	9.208	726	728	734	rBV	13339	12931	1.31%	0.086%
15	9.836	781	783	786	rVB	720823	652030	66.20%	4.325%
16	10.351	826	828	833	rVB2	38323	33370	3.39%	0.221%
17	10.648	852	854	857	rBV	342531	405215	41.14%	2.688%
18	11.334	912	914	916	rBV	12126	15903	1.61%	0.105%
19	11.551	932	933	936	rVB2	23741	29092	2.95%	0.193%
20	11.631	937	940	942	rBV	412744	428628	43.52%	2.843%
21	11.997	969	972	975	rBV2	9812	11365	1.15%	0.075%
22	12.351	1001	1003	1005	rVB	12879	11678	1.19%	0.077%
23	12.477	1012	1014	1016	rBV	376450	493395	50.09%	3.273%
24	12.511	1016	1017	1019	rVV	358881	266282	27.04%	1.766%
25	12.568	1019	1022	1024	rVV	39048	51593	5.24%	0.342%
26	12.625	1024	1027	1029	rVB3	9532	16109	1.64%	0.107%
27	12.785	1039	1041	1043	rBV	36575	34609	3.51%	0.230%
28	13.105	1067	1069	1071	rBV	29083	34671	3.52%	0.230%
29	13.139	1071	1072	1075	rVB	41877	38758	3.94%	0.257%
30	13.231	1078	1080	1082	rBV2	71917	98365	9.99%	0.653%
31	13.505	1100	1104	1106	rBV2	59012	84252	8.55%	0.559%
32	13.791	1126	1129	1131	rBV	13036	20593	2.09%	0.137%
33	13.882	1136	1137	1143	rVB2	17526	30939	3.14%	0.205%
34	13.974	1143	1145	1148	rBV	727702	766161	77.79%	5.083%

LSC Area Percent Report

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Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-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:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.054	1151	1152	1154	rVB2	13665	15428	1.57%	0.102%
36	14.088	1154	1155	1158	rBV	7440	11683	1.19%	0.078%
37	14.157	1158	1161	1162	rBV	32636	33170	3.37%	0.220%
38	14.248	1167	1169	1171	rBV	606630	696045	70.67%	4.617%
39	14.328	1173	1176	1177	rVB	15277	18907	1.92%	0.125%
40	14.351	1177	1178	1180	rVB	10362	10364	1.05%	0.069%
41	14.420	1182	1184	1186	rBV	23306	43756	4.44%	0.290%
42	14.477	1186	1189	1191	rVB	541243	677403	68.78%	4.494%
43	14.545	1191	1195	1196	rBV2	22596	49227	5.00%	0.327%
44	14.580	1196	1198	1200	rVB	12377	11717	1.19%	0.078%
45	14.671	1201	1206	1208	rBV	85324	140815	14.30%	0.934%
46	14.751	1211	1213	1215	rBV	64290	72923	7.40%	0.484%
47	14.797	1215	1217	1218	rBV	45953	52582	5.34%	0.349%
48	14.831	1218	1220	1222	rVB	30547	37478	3.81%	0.249%
49	14.877	1222	1224	1225	rBV	17086	17611	1.79%	0.117%
50	14.900	1225	1226	1228	rVB	14464	19164	1.95%	0.127%
51	14.945	1228	1230	1233	rBV	13771	26871	2.73%	0.178%
52	15.083	1240	1242	1243	rBV2	7866	11257	1.14%	0.075%
53	15.208	1251	1253	1254	rBV	16729	16329	1.66%	0.108%
54	15.254	1255	1257	1259	rVV3	16310	29799	3.03%	0.198%
55	15.300	1259	1261	1265	rVB	36246	56072	5.69%	0.372%
56	15.437	1270	1273	1274	rBV	55991	84292	8.56%	0.559%
57	15.471	1274	1276	1279	rBV3	48782	92653	9.41%	0.615%
58	15.517	1279	1280	1282	rBV2	24569	32055	3.25%	0.213%
59	15.563	1282	1284	1287	rVB	46573	63489	6.45%	0.421%
60	15.654	1289	1292	1295	rBV3	37702	101824	10.34%	0.675%
61	15.745	1295	1300	1302	rBV2	545254	984258	99.93%	6.529%
62	15.780	1302	1303	1305	rVB	323015	272522	27.67%	1.808%
63	15.825	1305	1307	1308	rVB2	27151	31539	3.20%	0.209%
64	15.871	1309	1311	1313	rVB	59772	73836	7.50%	0.490%
65	15.928	1314	1316	1317	rBV2	19331	22449	2.28%	0.149%
66	16.008	1321	1323	1325	rVB	34392	33264	3.38%	0.221%
67	16.054	1325	1327	1328	rBV2	34770	50363	5.11%	0.334%
68	16.248	1341	1344	1346	rBV	43290	72586	7.37%	0.482%
69	16.294	1346	1348	1351	rVV3	29983	50660	5.14%	0.336%
70	16.477	1361	1364	1366	rBV2	56660	87410	8.87%	0.580%
71	16.866	1396	1398	1401	rBV2	33240	53845	5.47%	0.357%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040815\
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Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-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:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	17.037	1411	1413	1418	rBV	333163	738893	75.02%	4.902%
73	17.266	1431	1433	1436	rBV	80018	122665	12.45%	0.814%
74	17.357	1439	1441	1444	rBV	220838	255655	25.96%	1.696%
75	17.414	1444	1446	1450	rVV	190372	269607	27.37%	1.789%
76	17.483	1450	1452	1457	rBV2	321418	511725	51.96%	3.395%
77	18.763	1562	1564	1569	rVB2	148979	291479	29.59%	1.934%
78	19.129	1593	1596	1601	rVB	115128	212536	21.58%	1.410%

Sum of corrected areas: 15074139

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040815\
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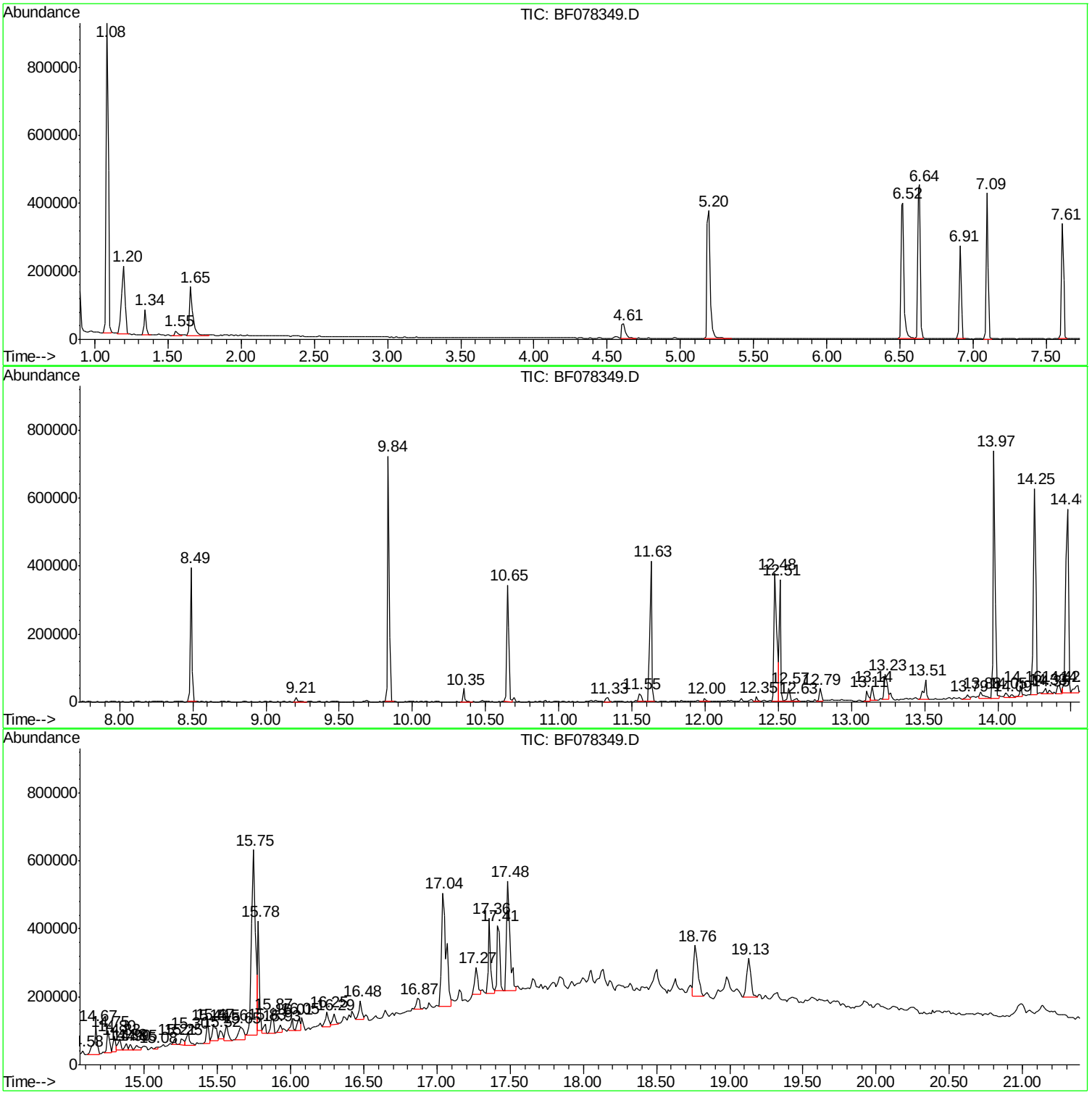
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

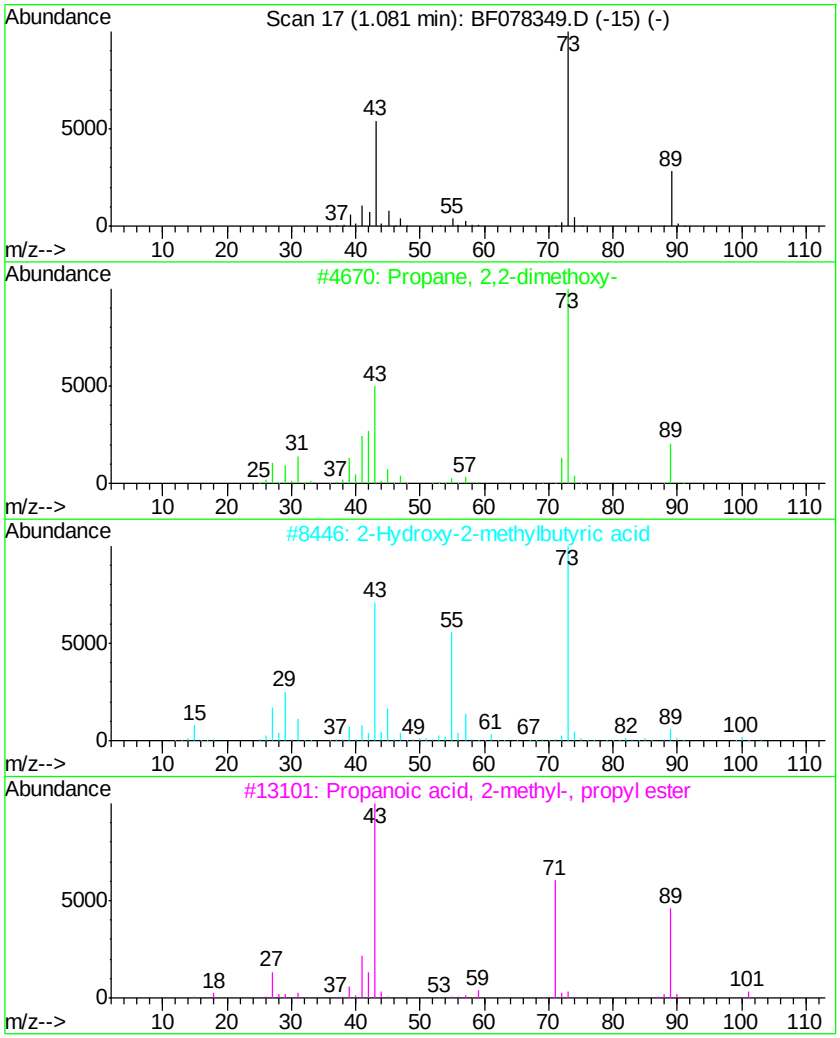
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

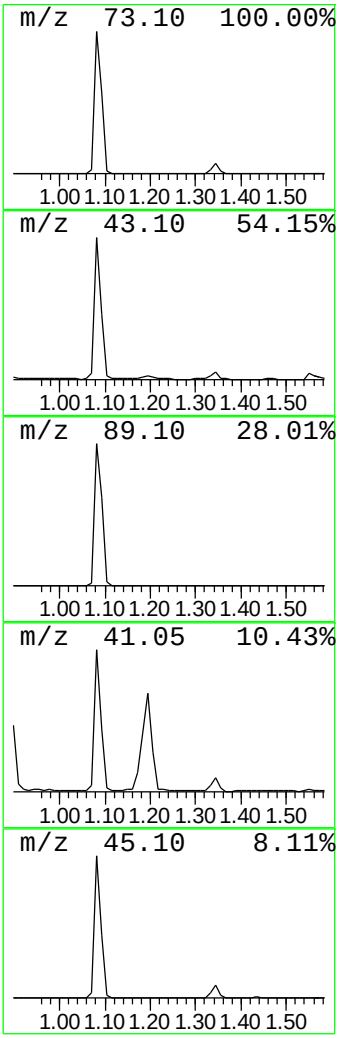
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.08	77.58 ng	984925	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





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Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

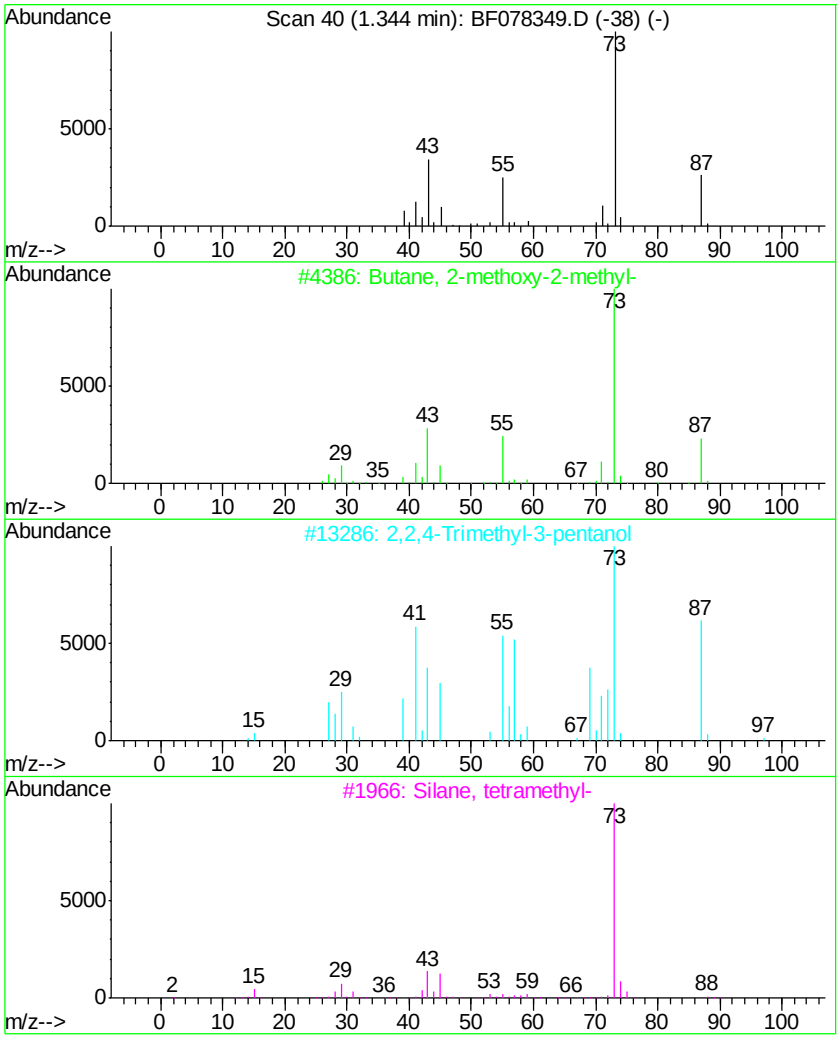
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

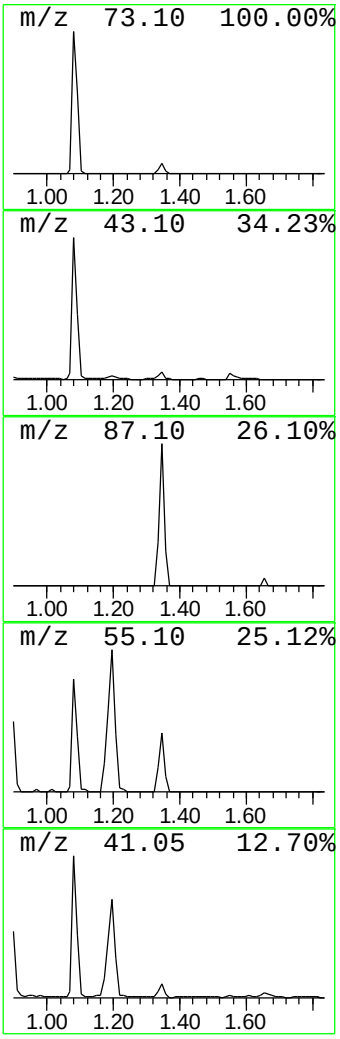
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.34	6.50 ng	82532	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040815\
Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

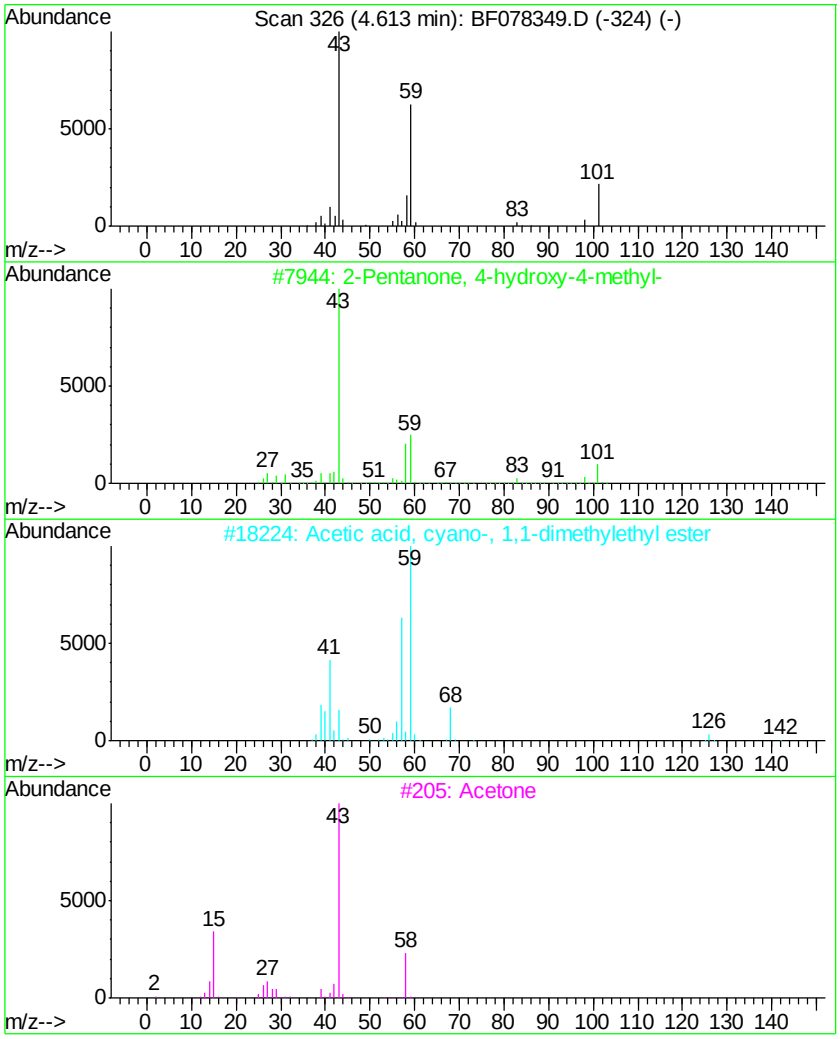
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

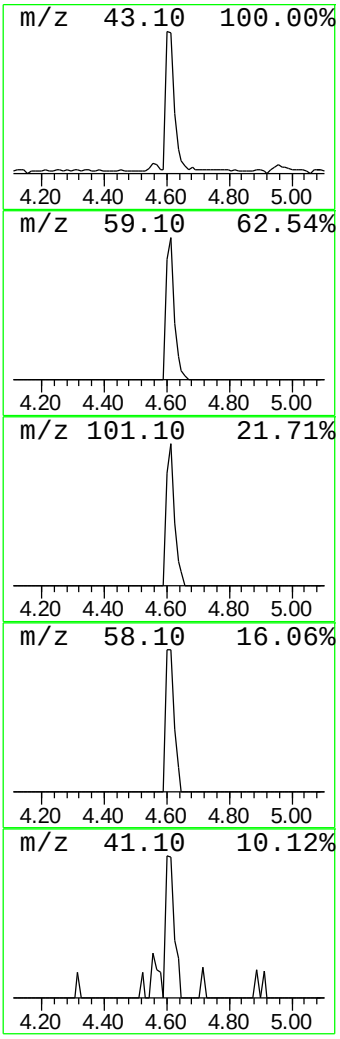
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	5.90 ng	74910	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Acetone	58	C3H6O	000067-64-1	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040815\
Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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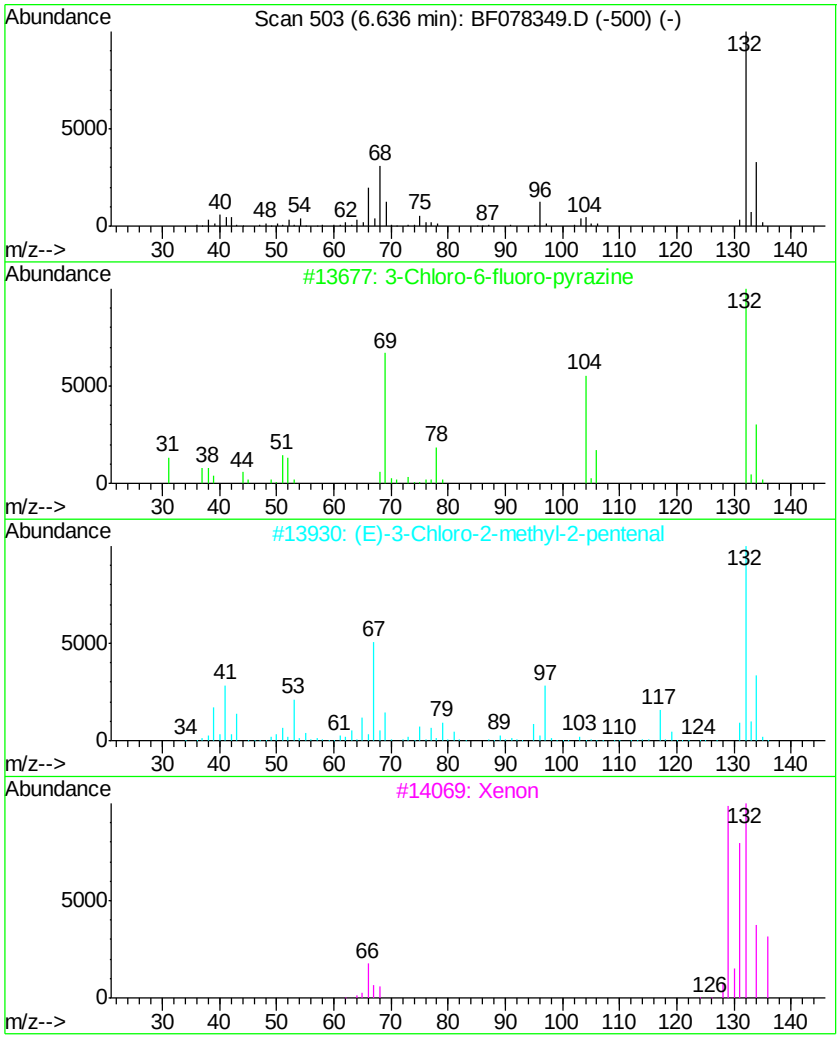
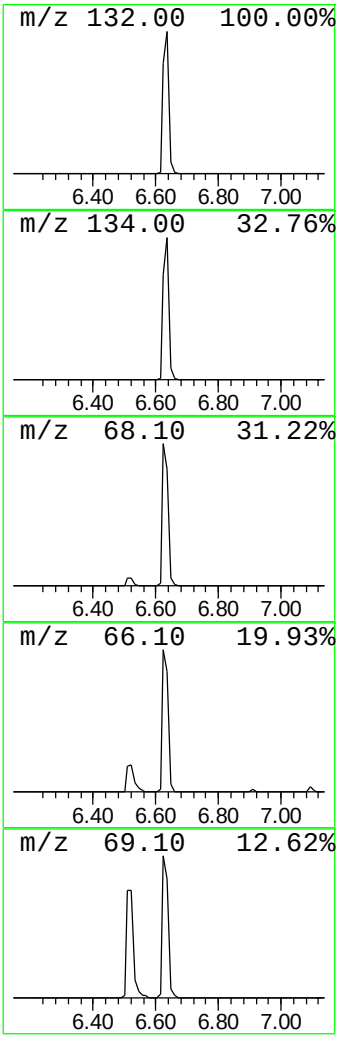
Peak Number 6 unknown6.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	50.23 ng	637767	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Xenon	132	Xe	007440-63-3	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Data File : BF078349.D
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Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

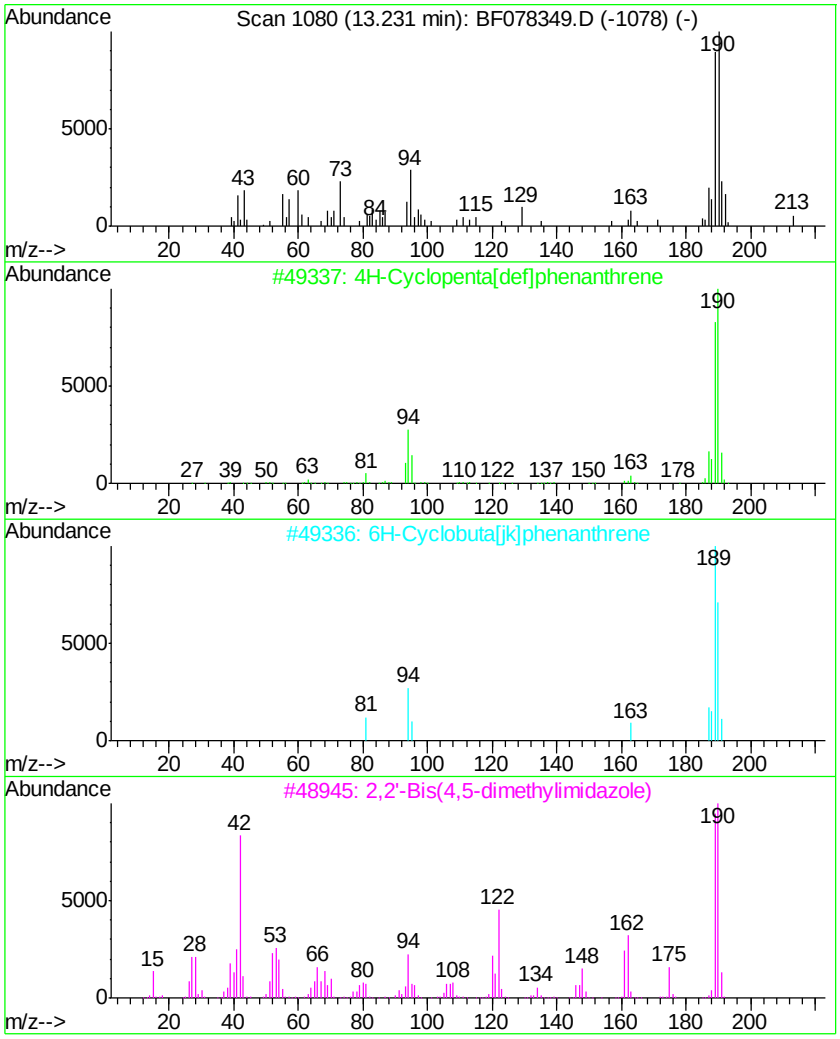
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

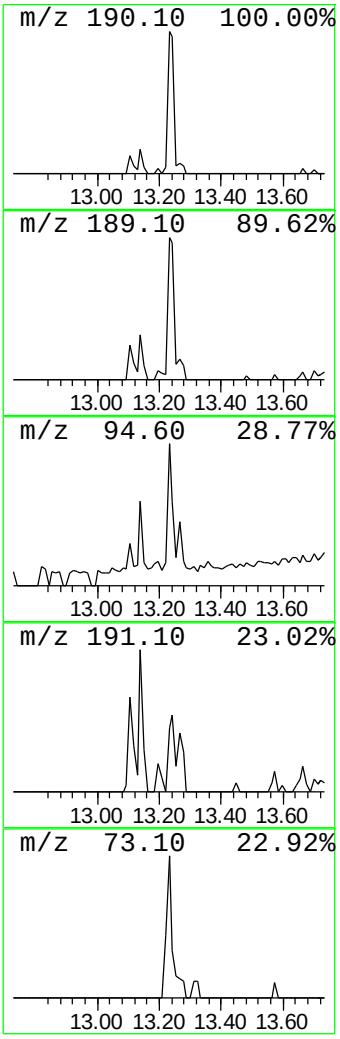
****

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	3.99 ng	98365	Phenanthrene-d10	12.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	36
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36
4	Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	28
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040815\
Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

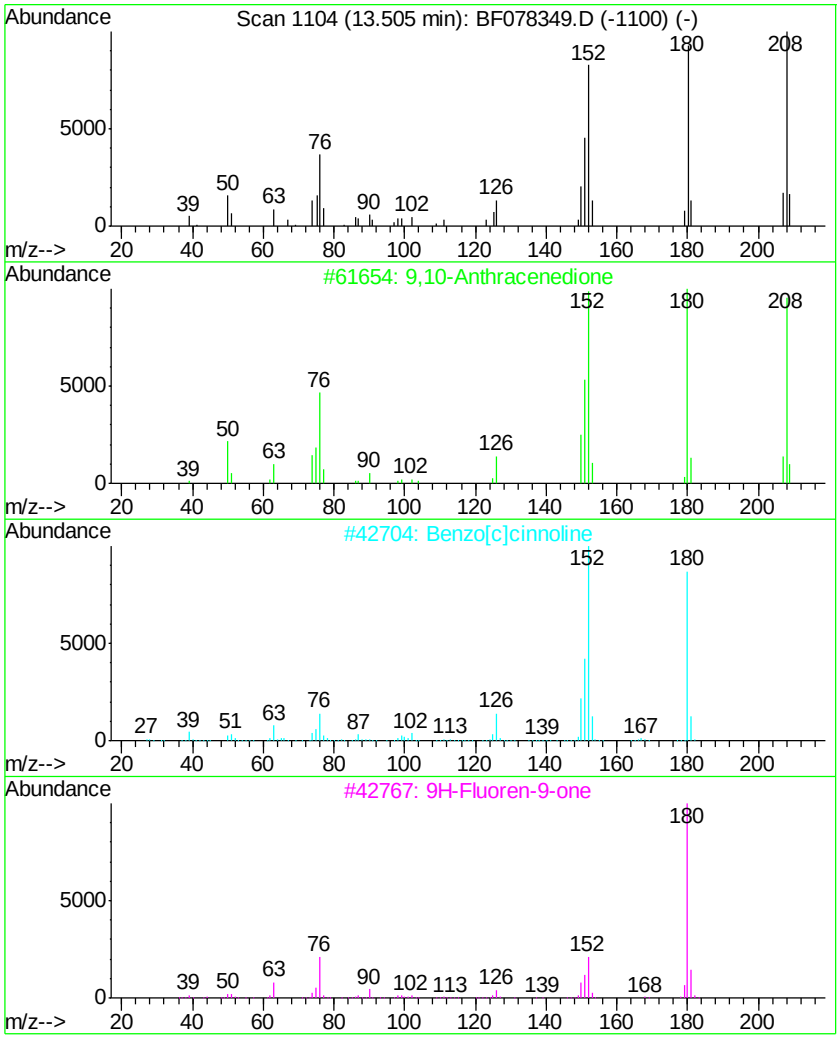
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

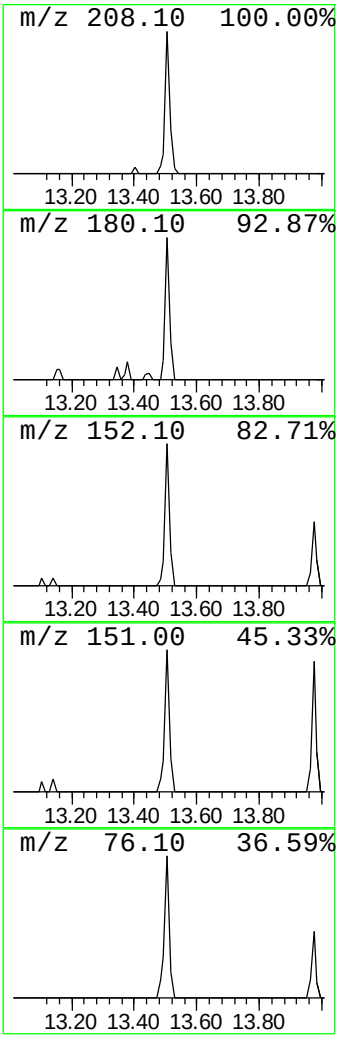
****

Peak Number 9 9,10-Anthracenedione Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	3.42 ng	84252	Phenanthrene-d10	12.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	92
3	9H-Fluoren-9-one	180	C13H8O	000486-25-9	70
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	60





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Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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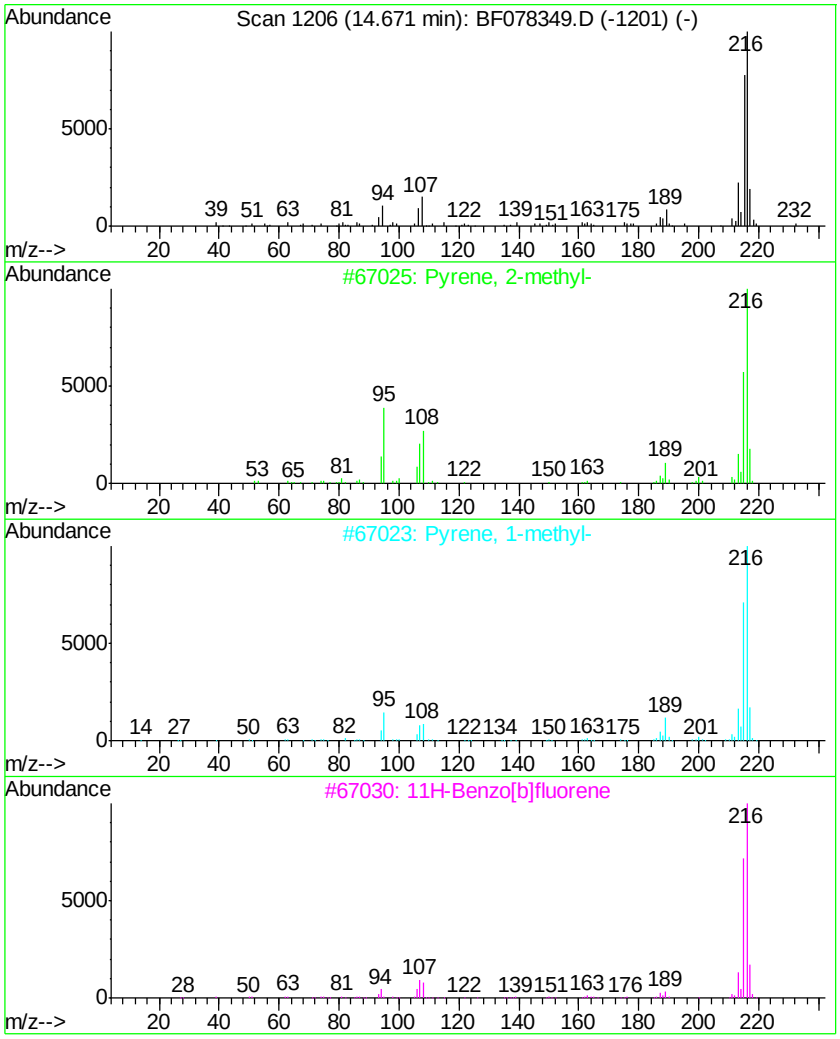
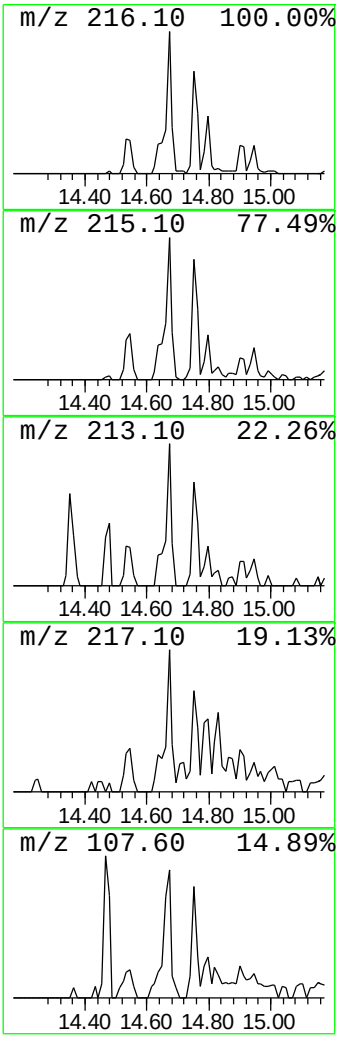
Peak Number 10 Pyrene, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.86 ng	140815	Chrysene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91





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Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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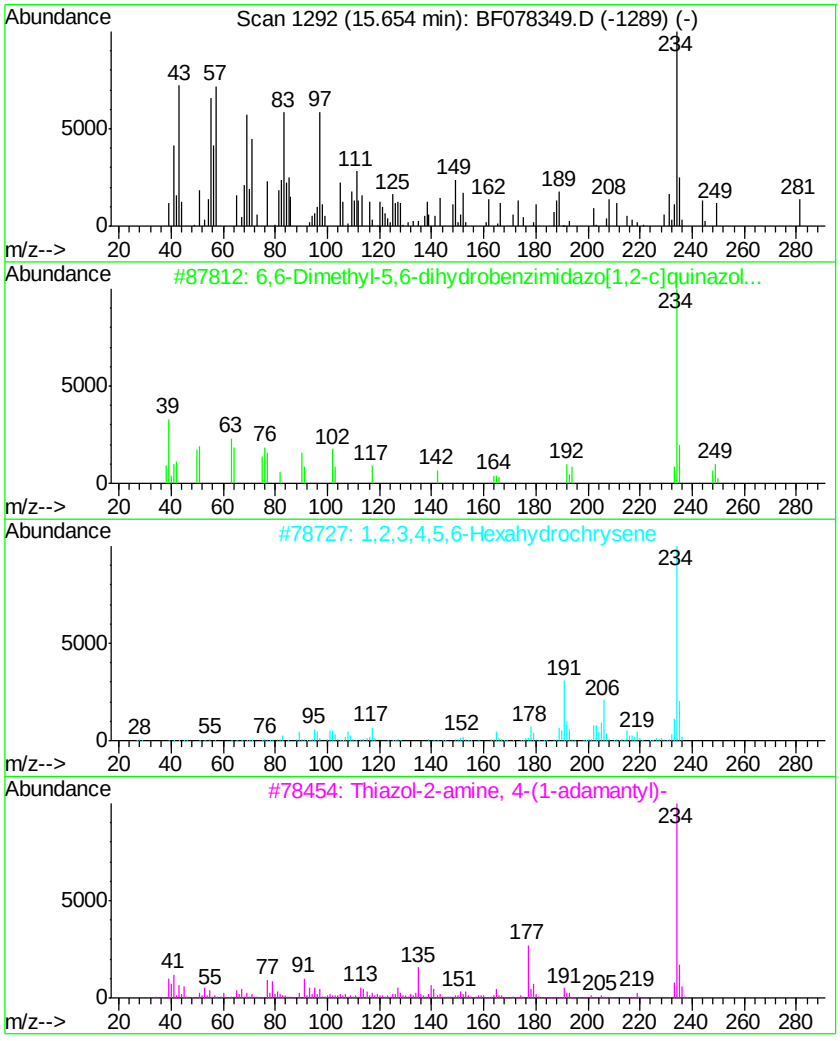
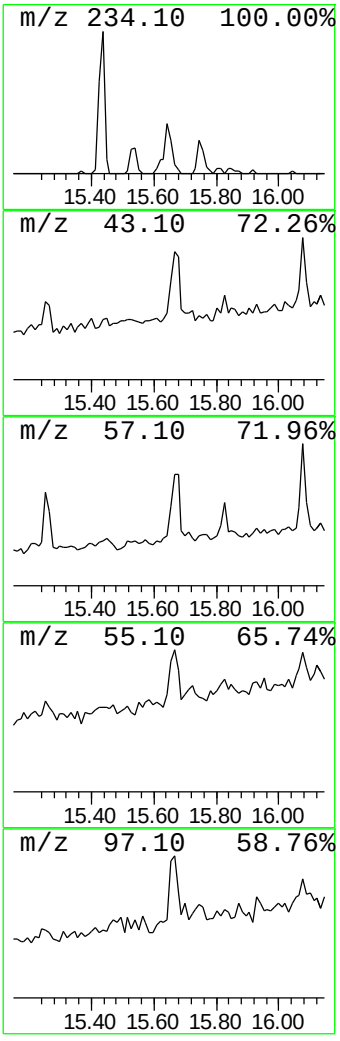
Peak Number 11 unknown15.65 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	2.07 ng	101824	Chrysene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,6-Dimethyl-5,6-dihydrobenzimid...	249	C16H15N3	060418-25-9	43
2	1,2,3,4,5,6-Hexahydrochrysene	234	C18H18	002091-91-0	43
3	Thiazol-2-amine, 4-(1-adamantyl)-	234	C13H18N2S	019735-74-1	38
4	Bicyclo[3.1.0]hexane, 1,6-diphenyl-	234	C18H18	056143-23-8	38
5	2,5-Diphenyl-2,4-hexadiene	234	C18H18	016819-47-9	38





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Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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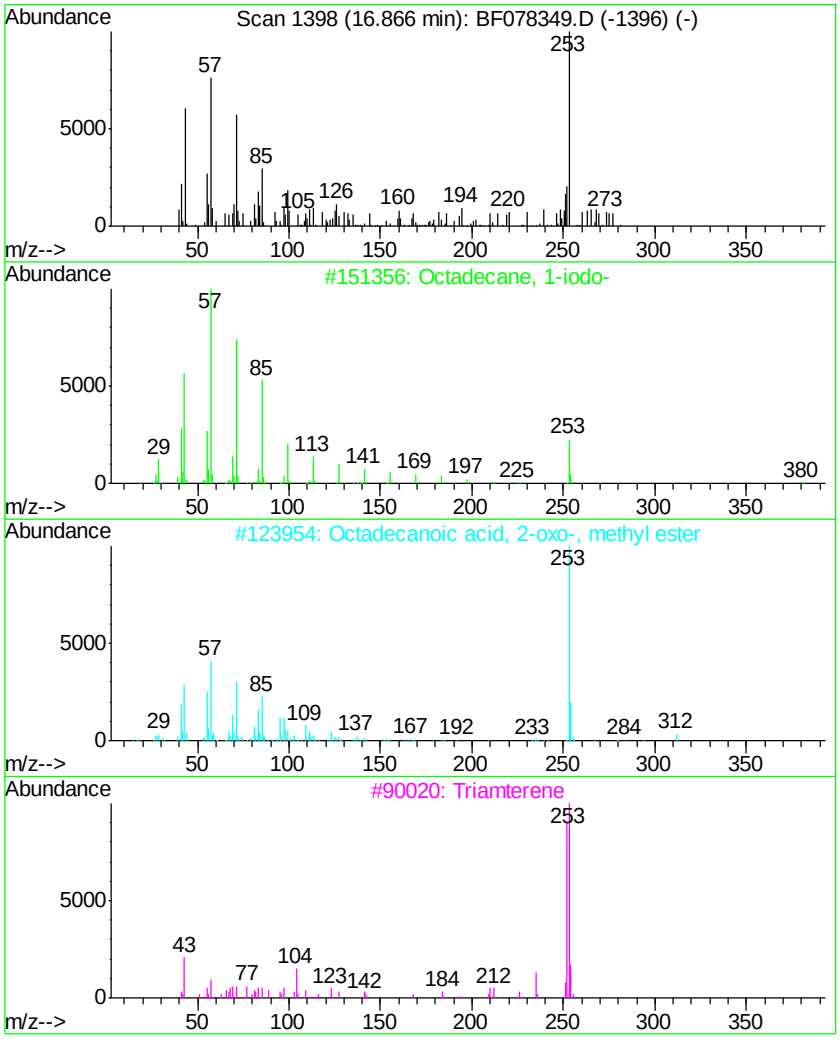
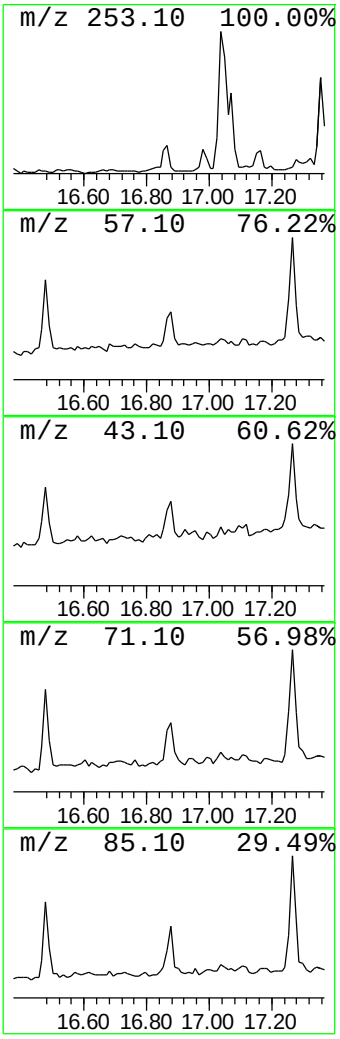
Peak Number 12 unknown16.87 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.87	2.10 ng	53845	Perylene-d12	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	42
2	Octadecanoic acid, 2-oxo-, methy...	312	C19H36O3	002380-18-9	38
3	Triamterene	253	C12H11N7	000396-01-0	35
4	1,2-Dihydrobenzo[b]fluoranthene	254	C20H14	100516-13-0	28
5	8-Chloro-5-methyl-2-phenylquinoline	253	C16H12ClN	025413-16-5	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040815\
Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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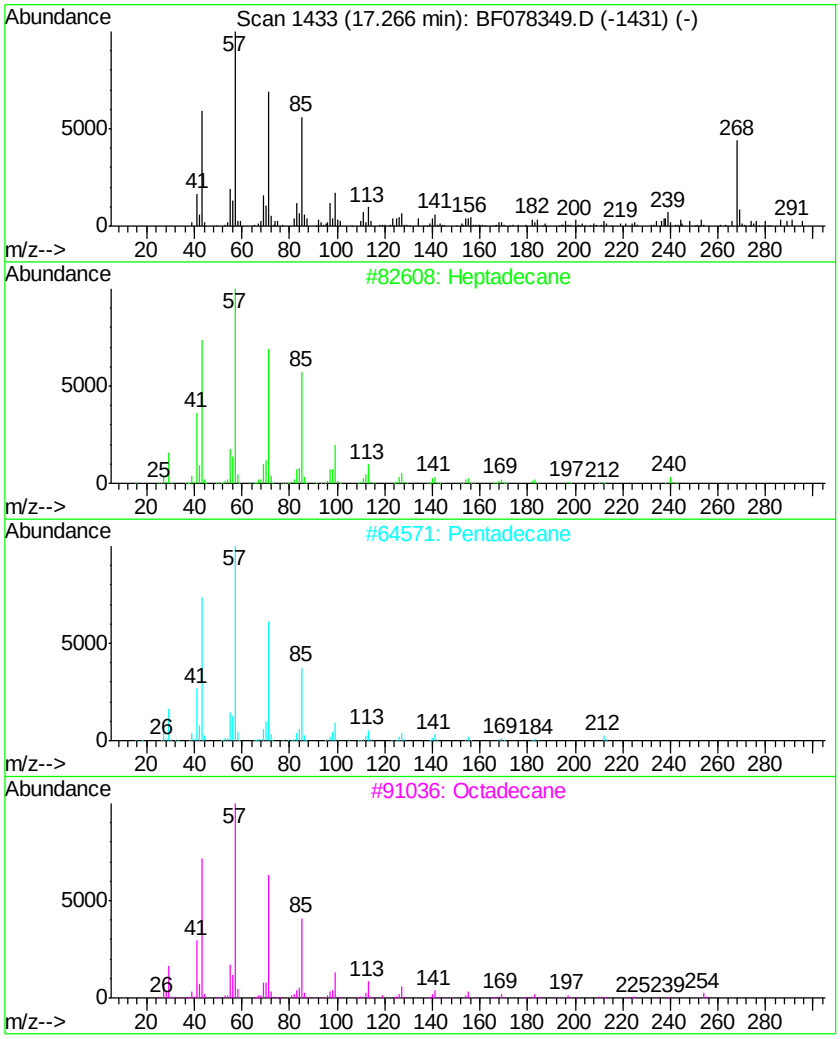
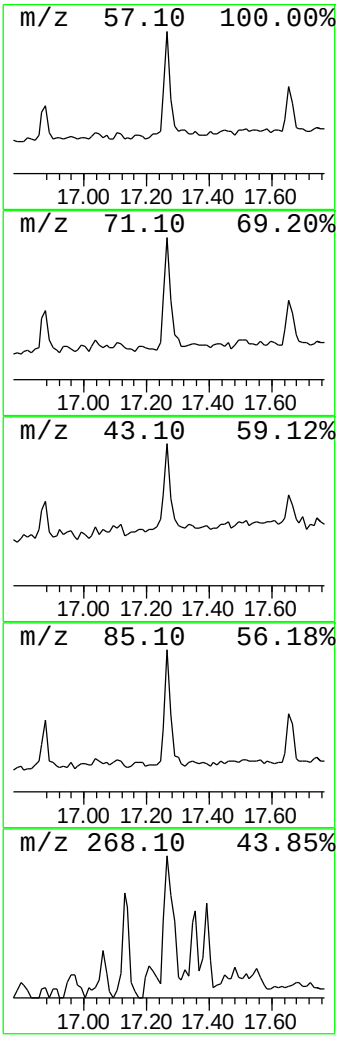
Peak Number 13 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	4.79 ng	122665	Perylene-d12	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Pentadecane	212	C15H32	000629-62-9	83
3	Octadecane	254	C18H38	000593-45-3	83
4	Octacosane	394	C28H58	000630-02-4	70
5	Tetracosane	338	C24H50	000646-31-1	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040815\
Data File : BF078349.D
Acq On : 8 Apr 2015 22:28
Operator : TP/IZ
Sample : G1794-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OUTFALL-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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
Propane, 2,2-dime...	1.08	77.6	ng	984925	1	6.91	253927	20.0
Butane, 2-methoxy...	1.34	6.5	ng	82532	1	6.91	253927	20.0
2-Pentanone, 4-hy...	4.61	5.9	ng	74910	1	6.91	253927	20.0
unknown6.64	6.64	50.2	ng	637767	1	6.91	253927	20.0
4H-Cyclopenta[def...	13.23	4.0	ng	98365	4	12.48	493395	20.0
9,10-Anthracenedione	13.51	3.4	ng	84252	4	12.48	493395	20.0
Pyrene, 2-methyl-	14.67	2.9	ng	140815	5	15.75	984258	20.0
unknown15.65	15.65	2.1	ng	101824	5	15.75	984258	20.0
unknown16.87	16.87	2.1	ng	53845	6	17.48	511725	20.0
Heptadecane	17.27	4.8	ng	122665	6	17.48	511725	20.0