LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104452.D
Acq On : 12 Apr 2018 15:48
Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

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-BF040618.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	5.040	497	502	512	rVB	139104	198242	5.25%	0.578%
2	5.434	558	569	571	rBV	3090091	3745370	99.20%	10.924%
3	5.751	619	623	629	rVB	49380	46125	1.22%	0.135%
4	6.451	730	742	745	rBV	3001485	3775690	100.00%	11.013%
5	6.581	759	764	767	rBV	3359276	3734342	98.90%	10.892%
6	6.810	799	803	807	rVB	1042937	832596	22.05%	2.428%
7	6.887	809	816	820	rBV	180222	190295	5.04%	0.555%
8	6.922	820	822	825	rVB	97170	76443	2.02%	0.223%
9	6.969	825	830	833	rBV	3192277	2928302	77.56%	8.541%
10	7.075	843	848	852	rVB4	37537	49974	1.32%	0.146%
11	7.210	867	871	873	rBV2	54111	52692	1.40%	0.154%
12	7.328	887	891	893	rBV3	35787	48314	1.28%	0.141%
13	7.381	894	900	902	rVB	2113534	2395068	63.43%	6.986%
14	7.451	908	912	915	rVB4	66647	86862	2.30%	0.253%
15	8.092	1015	1021	1023	rBV	1354098	1117768	29.60%	3.260%
16	8.116	1023	1025	1027	rVV	164637	136298	3.61%	0.398%
17	8.151	1027	1031	1033	rVV	65092	70943	1.88%	0.207%
18	8.181	1033	1036	1043	rVB7	28979	51209	1.36%	0.149%
19	8.292	1052	1055	1057	rVB	48131	40848	1.08%	0.119%
20	8.381	1063	1070	1072	rBV5	52372	78158	2.07%	0.228%
21	8.510	1089	1092	1094	rBV	104429	87416	2.32%	0.255%
22	8.628	1109	1112	1115	rBV3	45117	54664	1.45%	0.159%
23	8.681	1118	1121	1125	rVB3	46634	46986	1.24%	0.137%
24	8.775	1134	1137	1140	rVB3	36413	47972	1.27%	0.140%
25	8.869	1150	1153	1156	rBV5	29008	43044	1.14%	0.126%
26	9.034	1178	1181	1186	rBV4	27854	43717	1.16%	0.128%
27	9.110	1191	1194	1199	rVB	107907	89531	2.37%	0.261%
28	9.169	1199	1204	1207	rBV	3555831	3682240	97.52%	10.740%
29	9.245	1213	1217	1220	rBV	91358	102896	2.73%	0.300%
30	9.304	1225	1227	1232	rVB	95790	96714	2.56%	0.282%
31	9.563	1267	1271	1274	rBV	403371	404939	10.72%	1.181%
32	9.628	1278	1282	1284	rVB	230175	209831	5.56%	0.612%
33	9.710	1293	1296	1301	rBV4	88678	147364	3.90%	0.430%
34	9.757	1301	1304	1306	rVV	163023	146857	3.89%	0.428%

LSC Area Percent Report

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Acq On : 12 Apr 2018 15:48
Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.775	1306	1307	1309	rVV	85990	60002	1.59%	0.175%
36	9.810	1310	1313	1315	rVV	175031	168463	4.46%	0.491%
37	9.851	1316	1320	1323	rVV	1144928	1057724	28.01%	3.085%
38	9.881	1323	1325	1329	rVB2	88958	77062	2.04%	0.225%
39	10.104	1359	1363	1366	rBV3	67069	89000	2.36%	0.260%
40	10.169	1371	1374	1375	rBV2	68195	71798	1.90%	0.209%
41	10.216	1380	1382	1385	rBV3	57669	51893	1.37%	0.151%
42	10.257	1385	1389	1391	rBV2	221460	248141	6.57%	0.724%
43	10.281	1391	1393	1395	rVB	75493	64959	1.72%	0.189%
44	10.645	1450	1455	1457	rBV	1779115	1830091	48.47%	5.338%
45	10.763	1471	1475	1482	rVB3	206790	337948	8.95%	0.986%
46	11.339	1570	1573	1576	rBV	915312	844419	22.36%	2.463%
47	12.604	1786	1788	1791	rVB	608745	468972	12.42%	1.368%
48	12.939	1841	1845	1848	rVB	1840818	1780650	47.16%	5.194%
49	13.074	1865	1868	1870	rVB	531042	481476	12.75%	1.404%
50	13.992	2022	2024	2027	rVB	639675	535725	14.19%	1.563%
51	15.463	2270	2274	2284	rVB	518758	878683	23.27%	2.563%
52	16.580	2461	2464	2476	rVB2	187140	378359	10.02%	1.104%

Sum of corrected areas: 34285075

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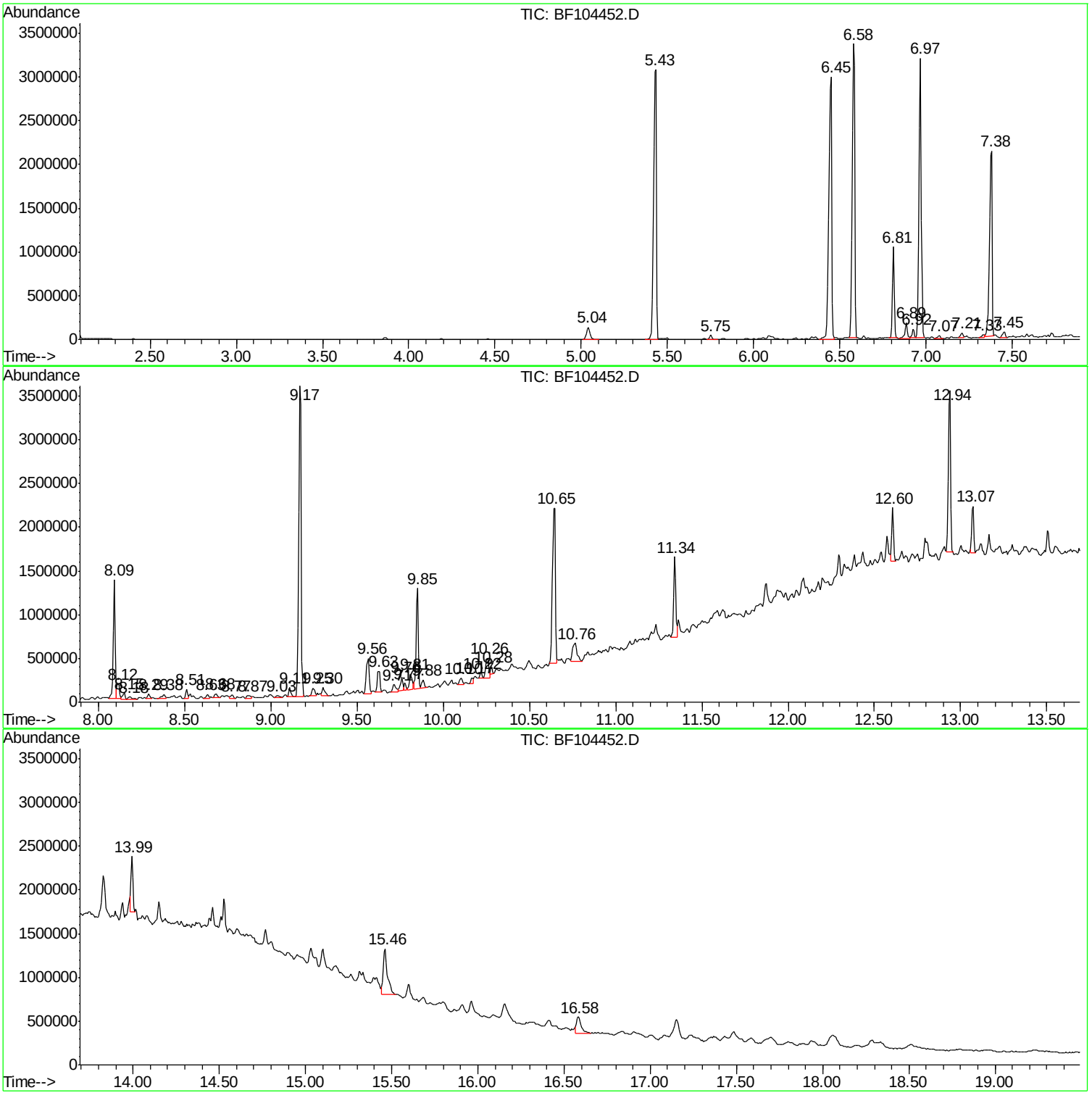
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF104452.D
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Operator : JU/SJ
Sample : J2335-05
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

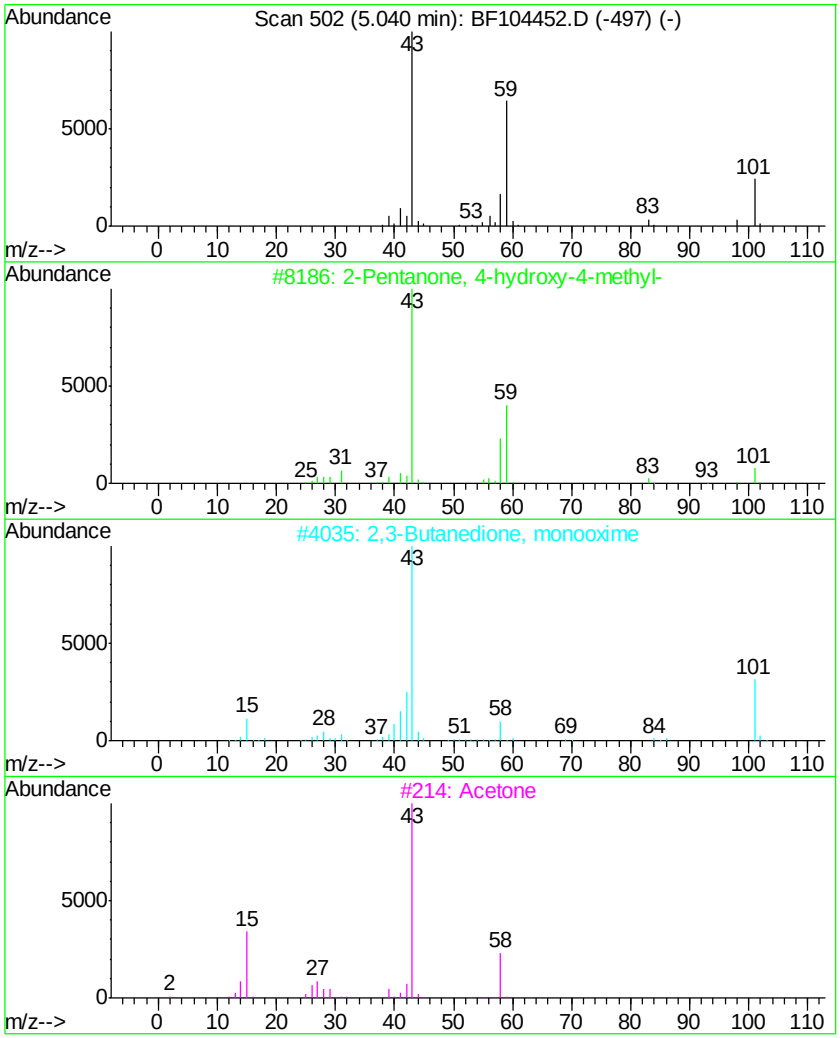
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

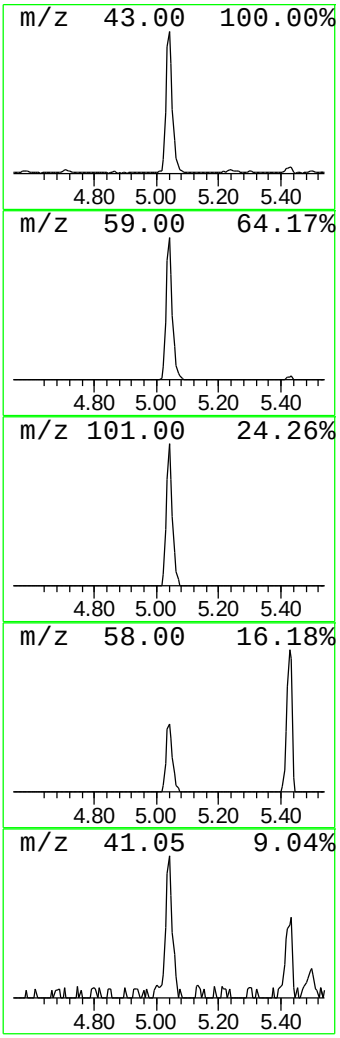
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.76 ng	198242	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetone	58	C3H6O	000067-64-1	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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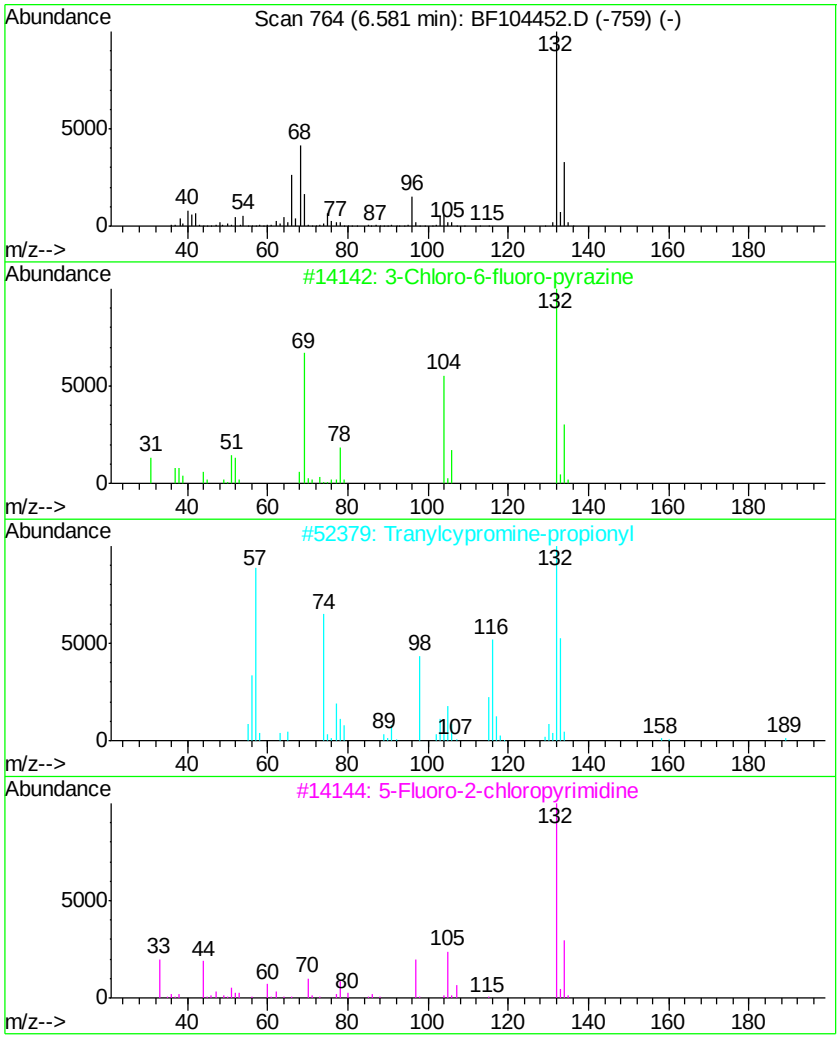
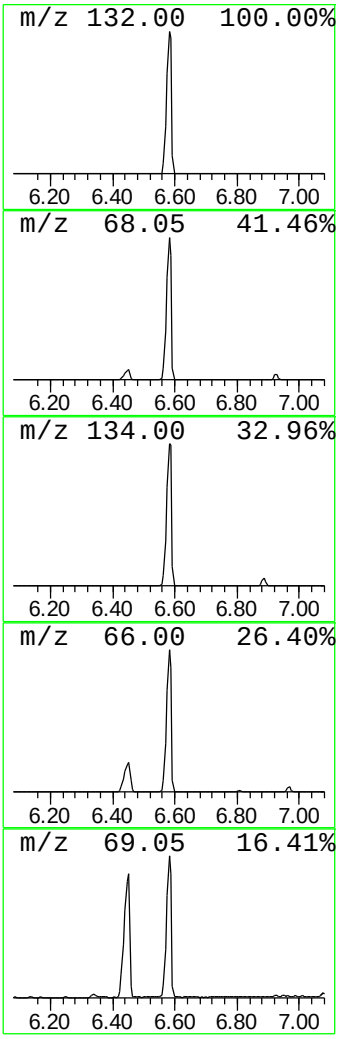
Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	89.70 ng	3734340	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104452.D
Acq On : 12 Apr 2018 15:48
Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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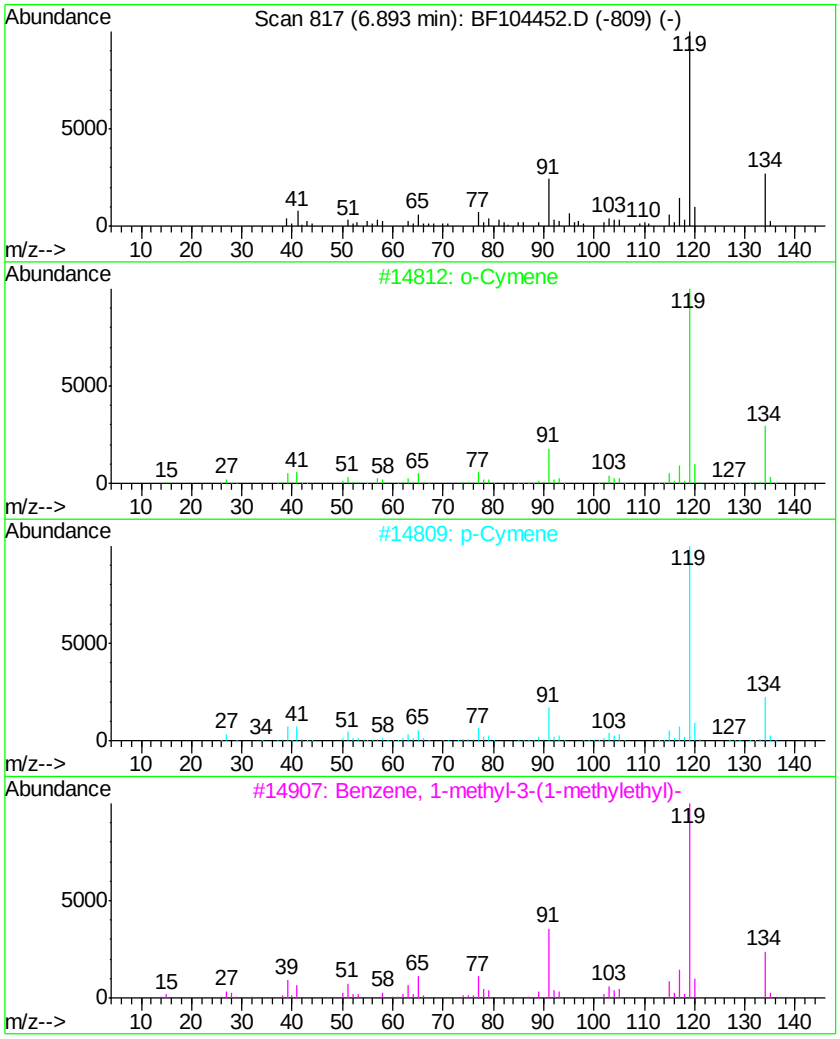
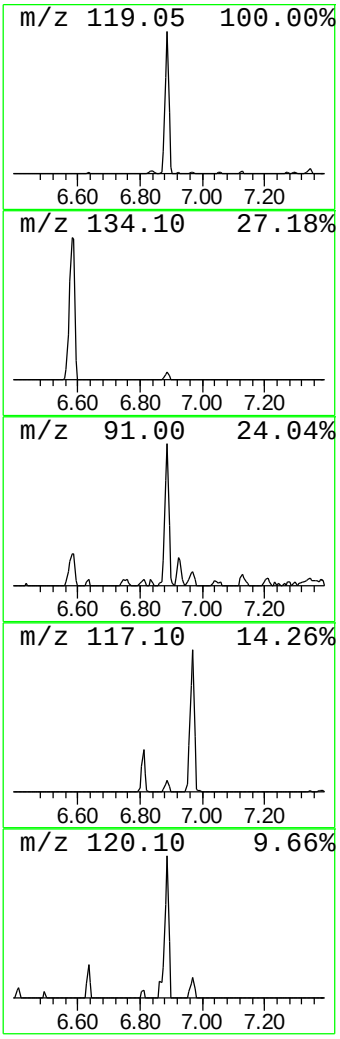
Peak Number 3 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.89	4.57 ng	190295	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	p-Cymene	134	C10H14	000099-87-6	97
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87





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Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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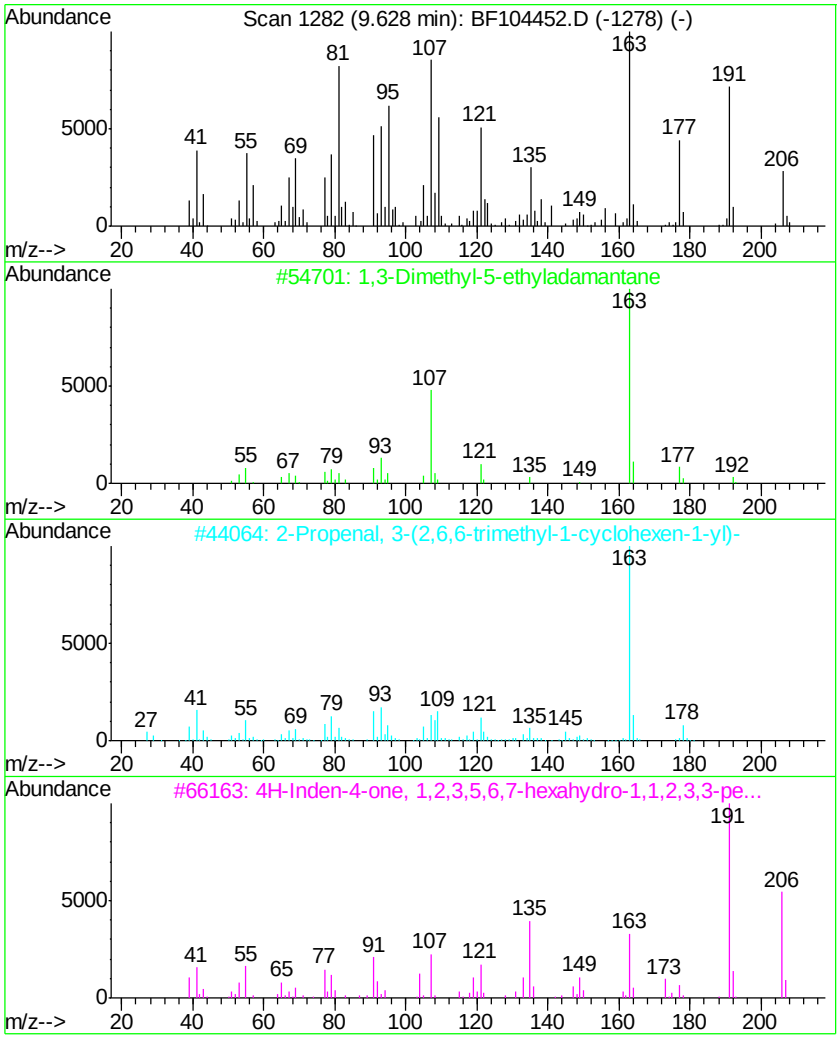
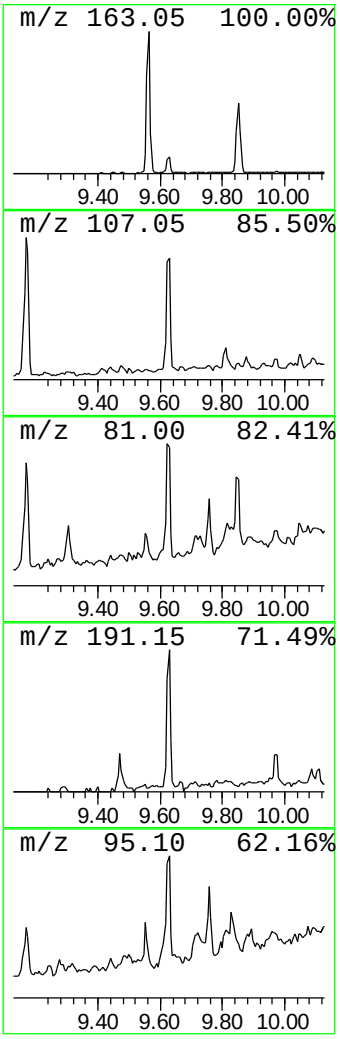
Peak Number 5 unknown9.63 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	3.97 ng	209831	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	38
2	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	27
3	4H-Inden-4-one, 1,2,3,5,6,7-hexa...	206	C14H22O	033704-61-9	25
4	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	22
5	3,7,11,Trimethyl-8,10- dodecedie...	266	C17H30O2	1000374-10-3	14





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Sample : J2335-05
Misc :
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Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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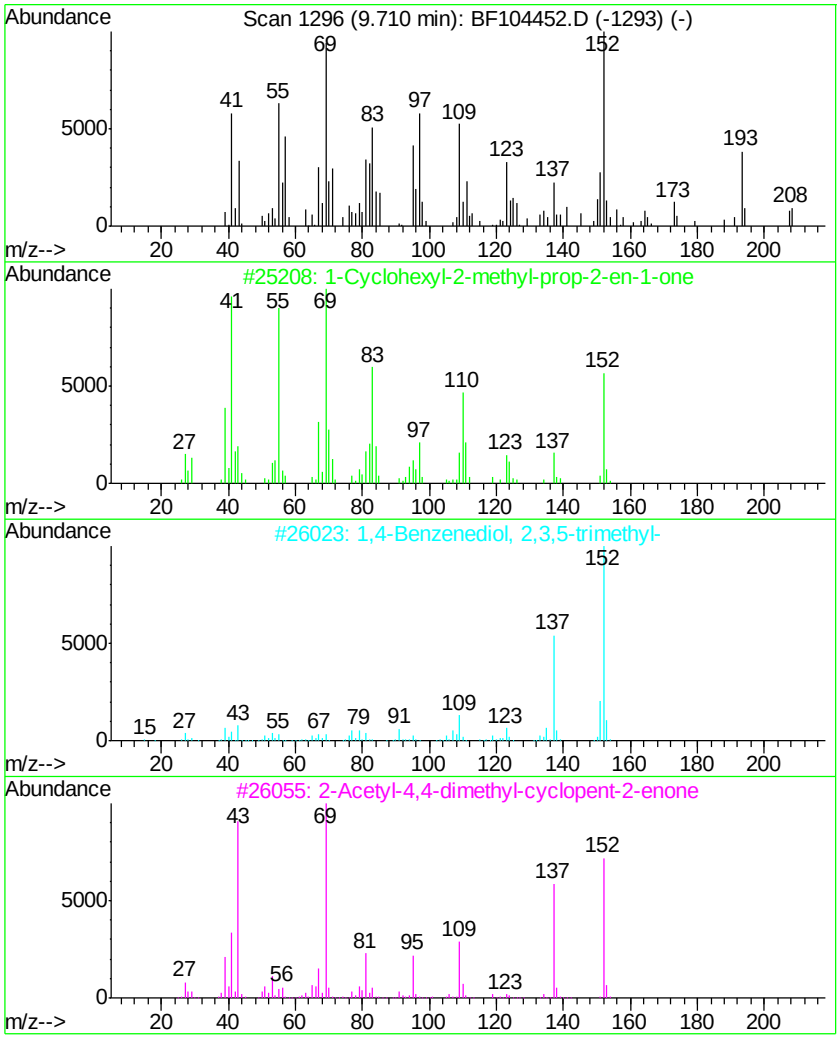
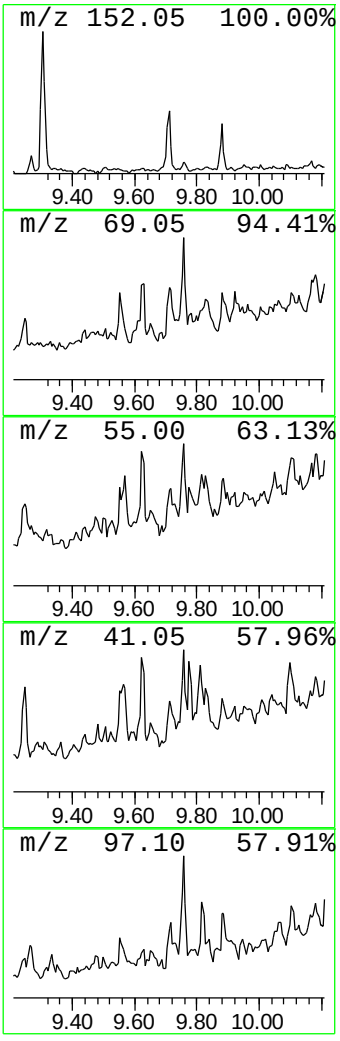
Peak Number 6 1-Cyclohexyl-2-methyl-prop-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.71	2.79 ng	147364	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexyl-2-methyl-prop-2-en-...	152	C10H16O	025183-82-8	55
2	1,4-Benzenediol, 2,3,5-trimethyl-	152	C9H12O2	000700-13-0	30
3	2-Acetyl-4,4-dimethyl-cyclopent-...	152	C9H12O2	081979-96-6	30
4	2H-Pyrrol-2-one, 1,5-dihydro-4-(...	152	C8H12N2O	105776-93-0	25
5	4H-1-Benzothiopyran-4-one, 2,3-d...	194	C10H10O2S	029373-04-4	18





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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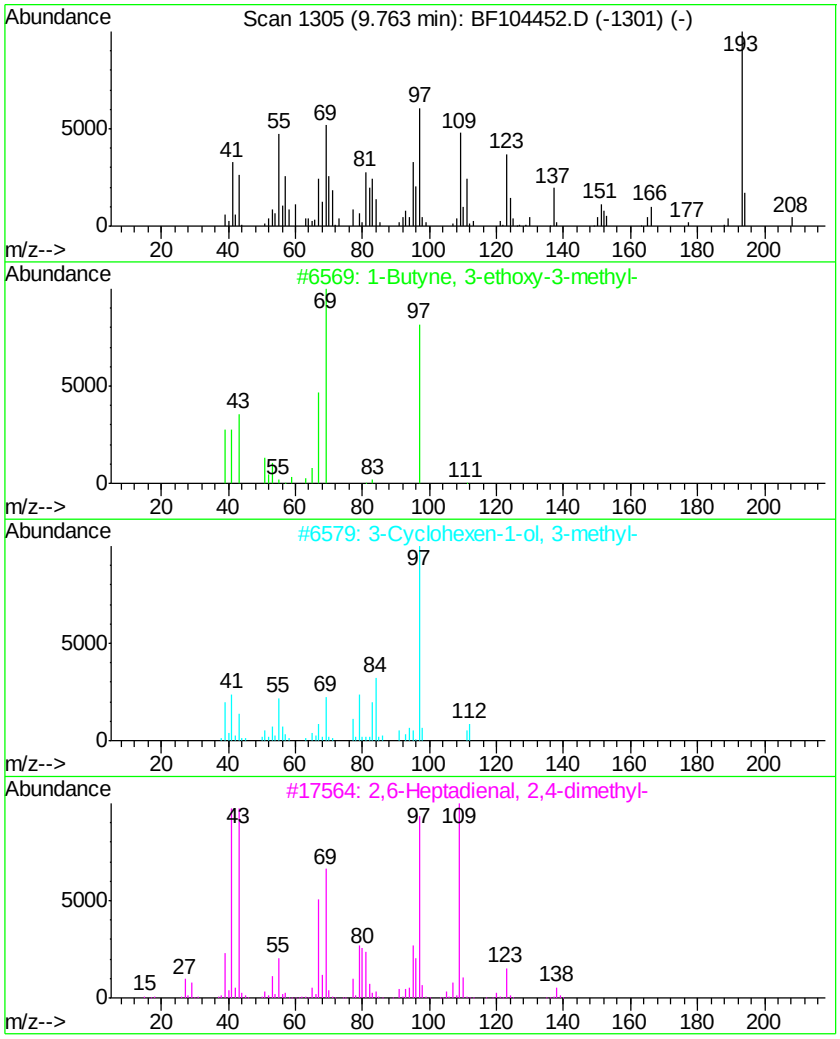
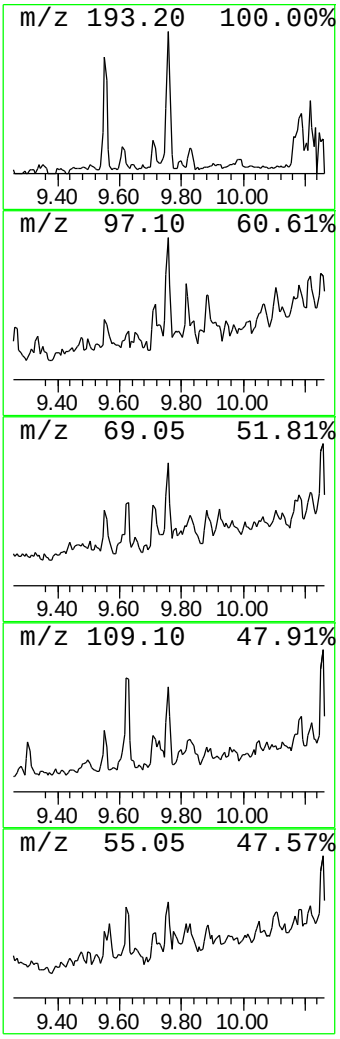
Peak Number 7 unknown9.76 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.78 ng	146857	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butyne, 3-ethoxy-3-methyl-	112	C7H12O	007740-69-4	27
2	3-Cyclohexen-1-ol, 3-methyl-	112	C7H12O	053783-91-8	27
3	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
4	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
5	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054824-04-3	18





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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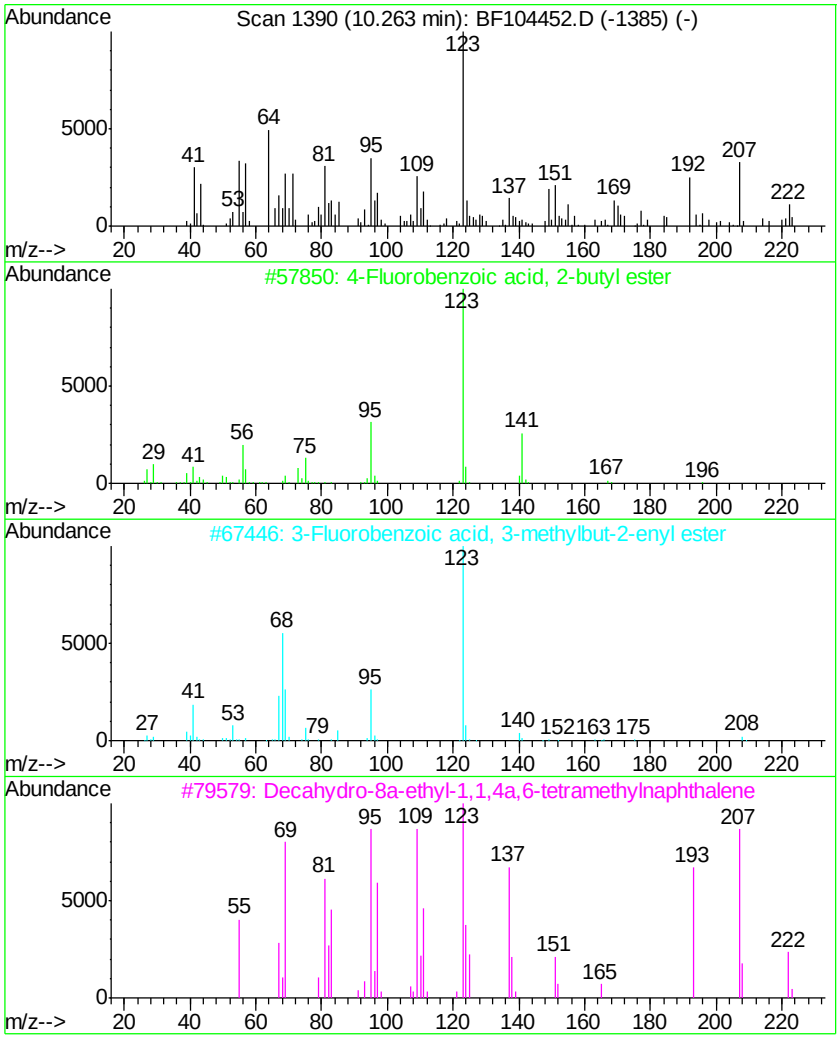
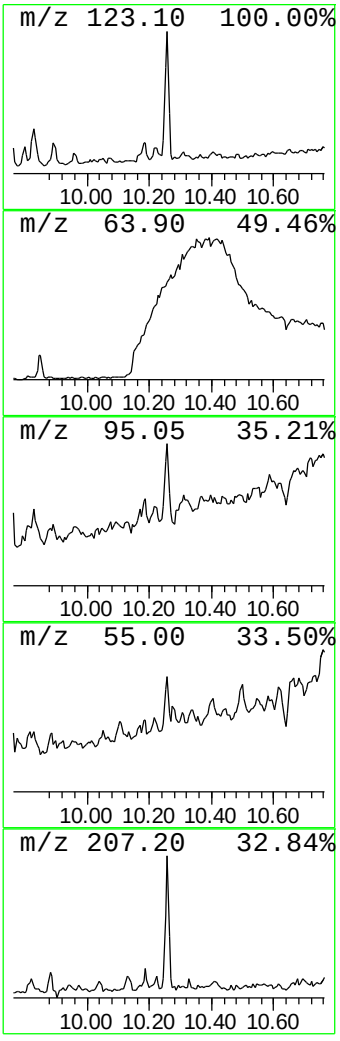
Peak Number 8 unknown10.26 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	4.69 ng	248141	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluorobenzoic acid, 2-butyl ester	196	C11H13FO2	090172-12-6	46
2	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	46
3	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	43
4	3-Fluorobenzoic acid, 3-chloropr...	214	C10H8ClFO2	1000292-61-0	43
5	2-Fluorobenzoic acid, 4-tetradec...	336	C21H33FO2	1000280-61-4	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104452.D
Acq On : 12 Apr 2018 15:48
Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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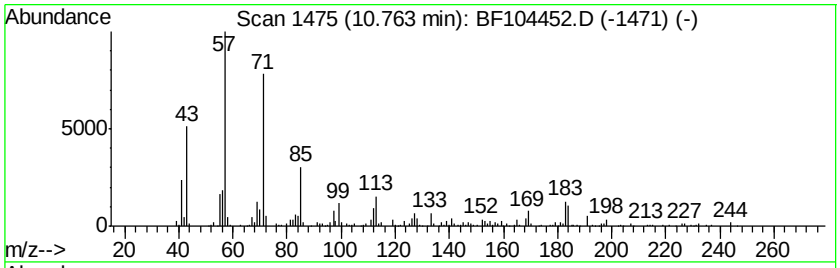
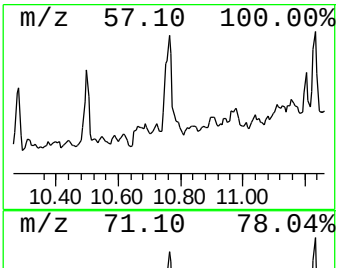
Peak Number 9 Pentadecane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	8.00 ng	337948	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 4-methyl-	226	C16H34	002801-87-8	91
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	87
3	Decane, 2-methyl-	156	C11H24	006975-98-0	81
4	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	81
5	Heptacosane	380	C27H56	000593-49-7	72





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Data File : BF104452.D
Acq On : 12 Apr 2018 15:48
Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

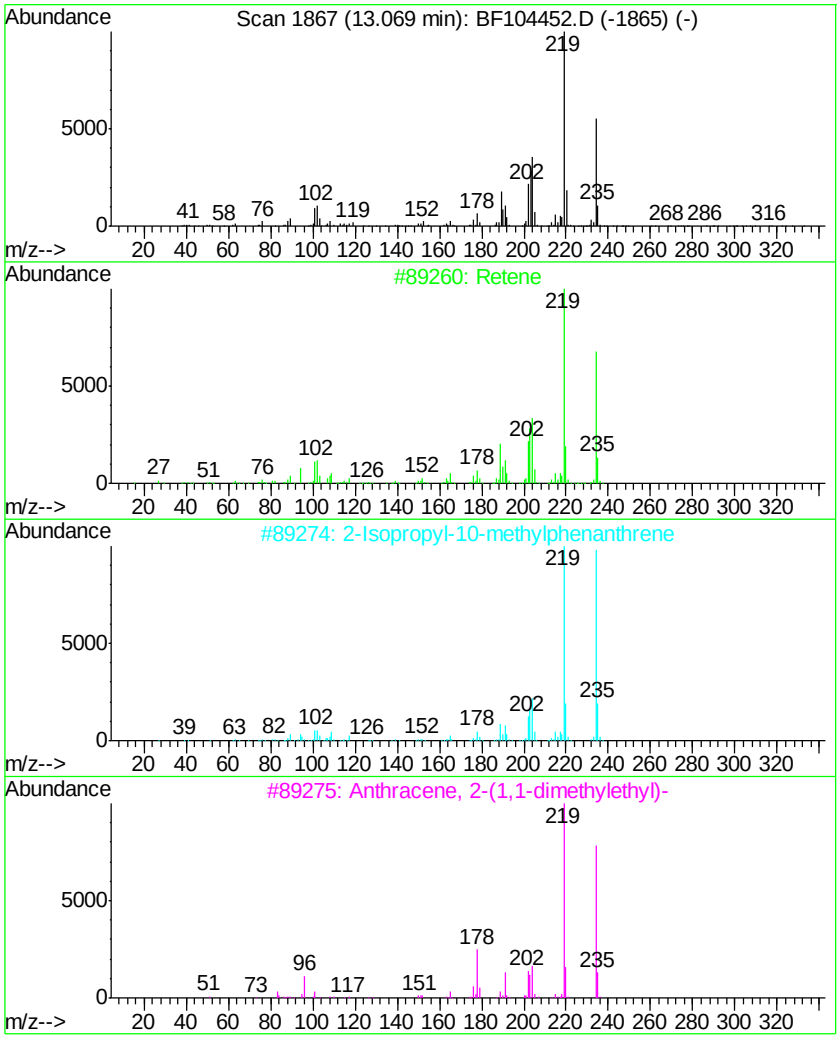
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

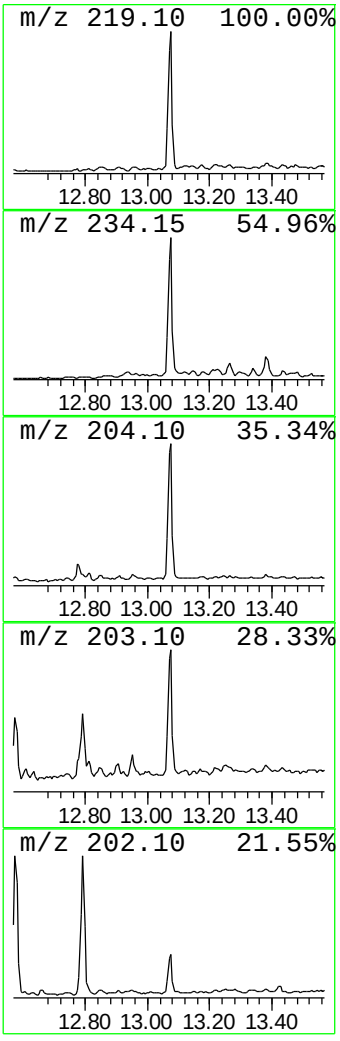
****

Peak Number 10 Retene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	17.97 ng	481476	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Retene	234	C18H18	000483-65-8	98
2	2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	95
3	Anthracene, 2-(1,1-dimethylethyl)-	234	C18H18	018801-00-8	80
4	Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	76
5	Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104452.D
Acq On : 12 Apr 2018 15:48
Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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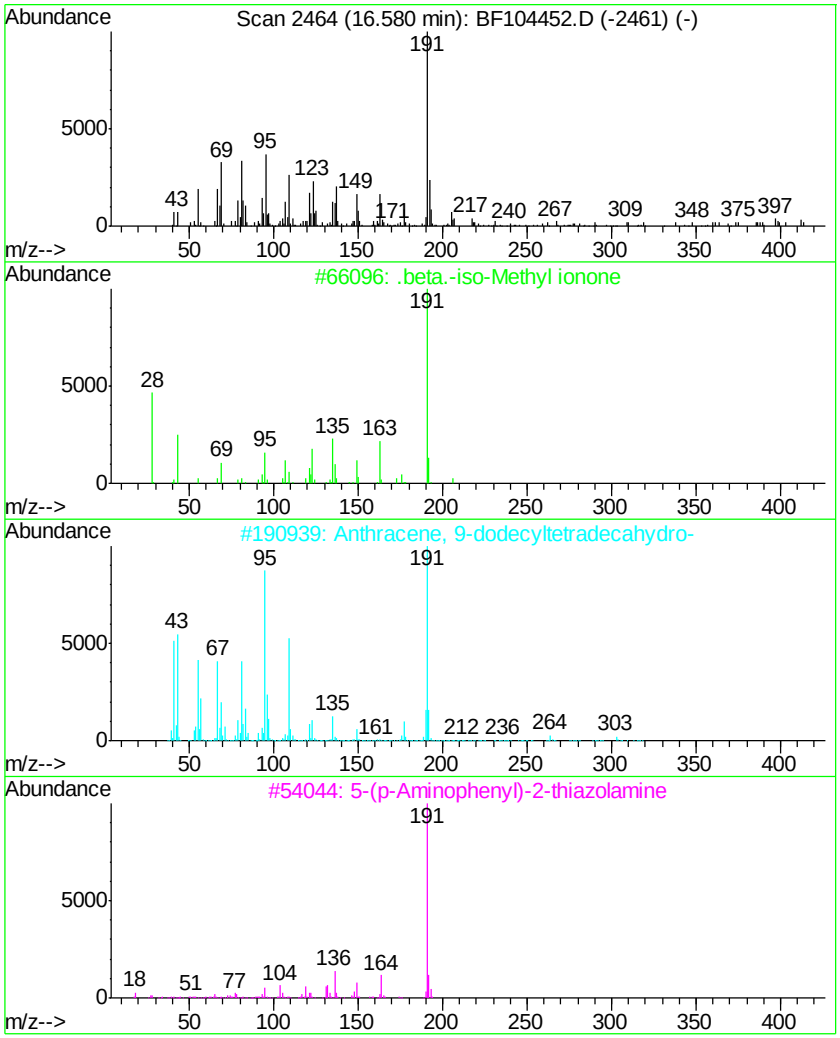
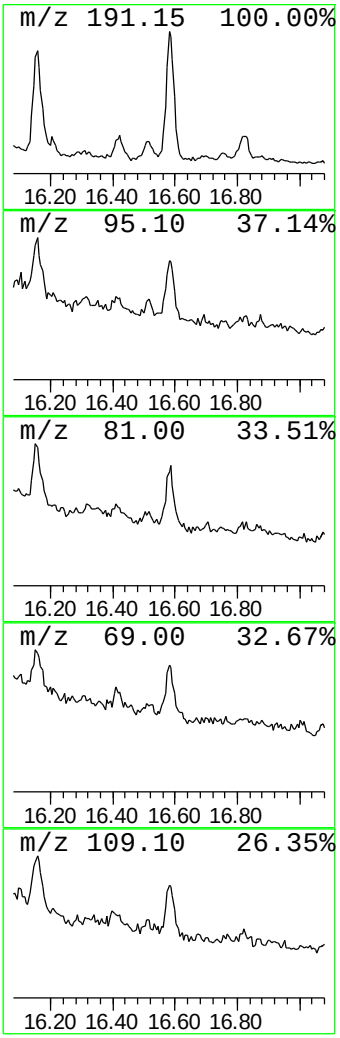
Peak Number 11 .beta.-iso-Methyl ionone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	8.61 ng	378359	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	42
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	38
4	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	38
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041218\
Data File : BF104452.D
Acq On : 12 Apr 2018 15:48
Operator : JU/SJ
Sample : J2335-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.04	4.8	ng	198242	1	6.81	832596	20.0
unknown6.58	6.58	89.7	ng	3734340	1	6.81	832596	20.0
o-Cymene	6.89	4.6	ng	190295	1	6.81	832596	20.0
unknown9.63	9.63	4.0	ng	209831	3	9.85	1057720	20.0
1-Cyclohexyl-2-me...	9.71	2.8	ng	147364	3	9.85	1057720	20.0
unknown9.76	9.76	2.8	ng	146857	3	9.85	1057720	20.0
unknown10.26	10.26	4.7	ng	248141	3	9.85	1057720	20.0
Pentadecane, 4-me...	10.76	8.0	ng	337948	4	11.34	844419	20.0
Retene	13.07	18.0	ng	481476	5	13.99	535725	20.0
.beta.-iso-Methyl...	16.58	8.6	ng	378359	6	15.46	878683	20.0