LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109148.D
Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

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_F\METHODS\8270-BF091418.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	4.907	434	437	444	rVB	78312	86440	1.27%	0.214%
2	5.331	505	509	518	rBV	1310690	1360104	19.94%	3.362%
3	6.354	679	683	690	rBV2	981790	947811	13.89%	2.343%
4	6.490	702	706	710	rBV	2493697	2332492	34.19%	5.765%
5	6.725	742	746	749	rBV	1016716	918082	13.46%	2.269%
6	6.878	768	772	776	rVB	2396690	2220308	32.55%	5.488%
7	7.119	806	813	821	rBV2	333538	736133	10.79%	1.820%
8	7.284	835	841	844	rBV	1901753	1803713	26.44%	4.458%
9	7.748	916	920	924	rBV4	72967	90392	1.33%	0.223%
10	8.001	959	963	966	rBV	1279135	1073716	15.74%	2.654%
11	8.278	1007	1010	1012	rVV	555077	467271	6.85%	1.155%
12	8.295	1012	1013	1018	rVB	160105	141926	2.08%	0.351%
13	8.342	1018	1021	1023	rBV4	81359	75775	1.11%	0.187%
14	8.419	1031	1034	1036	rBV	229850	185335	2.72%	0.458%
15	8.584	1055	1062	1065	rBV2	463775	469929	6.89%	1.162%
16	8.931	1119	1121	1123	rBV	79028	73829	1.08%	0.182%
17	9.083	1142	1147	1148	rBV	3341998	3249258	47.63%	8.032%
18	9.095	1148	1149	1152	rVB	2259822	1496383	21.94%	3.699%
19	9.166	1158	1161	1166	rBV4	173440	197660	2.90%	0.489%
20	9.401	1197	1201	1205	rVV6	109201	178270	2.61%	0.441%
21	9.448	1206	1209	1211	rVV2	122706	130075	1.91%	0.322%
22	9.472	1211	1213	1218	rVB	527152	412545	6.05%	1.020%
23	9.548	1223	1226	1228	rVB2	88552	80159	1.18%	0.198%
24	9.754	1257	1261	1265	rBV	1219945	1045550	15.33%	2.584%
25	9.919	1285	1289	1292	rVB	1153110	995538	14.59%	2.461%
26	9.983	1297	1300	1303	rVB	117078	99879	1.46%	0.247%
27	10.172	1329	1332	1335	rBV2	63659	71295	1.05%	0.176%
28	10.436	1375	1377	1379	rBV	131879	98058	1.44%	0.242%
29	10.483	1379	1385	1387	rVV	6050975	6821284	100.00%	16.861%
30	10.542	1387	1395	1398	rVV	1616620	1475853	21.64%	3.648%
31	10.607	1402	1406	1409	rVB	1325801	1019007	14.94%	2.519%
32	10.642	1410	1412	1415	rBV	101731	95219	1.40%	0.235%
33	10.677	1415	1418	1421	rVB3	85030	101857	1.49%	0.252%
34	10.730	1424	1427	1429	rVV	239130	258183	3.78%	0.638%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

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_F\METHODS\8270-BF091418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.754	1429	1431	1436	rVB4	425875	376143	5.51%	0.930%
36	10.860	1446	1449	1454	rVB4	83349	119889	1.76%	0.296%
37	10.919	1454	1459	1461	rBV4	53994	90530	1.33%	0.224%
38	11.230	1509	1512	1515	rBV	1005880	837389	12.28%	2.070%
39	11.407	1540	1542	1547	rVB	203404	161646	2.37%	0.400%
40	11.524	1559	1562	1564	rBV	417906	323397	4.74%	0.799%
41	11.554	1564	1567	1572	rVB2	184159	177647	2.60%	0.439%
42	11.777	1602	1605	1613	rBV	470934	539954	7.92%	1.335%
43	11.942	1630	1633	1637	rBV	195427	174035	2.55%	0.430%
44	12.330	1696	1699	1703	rVB	202234	175215	2.57%	0.433%
45	12.436	1714	1717	1720	rVB	182678	143247	2.10%	0.354%
46	12.536	1730	1734	1736	rBV	478976	523104	7.67%	1.293%
47	12.560	1736	1738	1742	rVB	193754	185971	2.73%	0.460%
48	12.766	1771	1773	1777	rBV2	59792	69762	1.02%	0.172%
49	12.813	1777	1781	1785	rVB	2454955	2427378	35.59%	6.000%
50	13.383	1876	1878	1886	rVB3	65310	80540	1.18%	0.199%
51	13.724	1933	1936	1944	rVB2	210302	250967	3.68%	0.620%
52	13.860	1955	1959	1962	rBV	1189066	1105493	16.21%	2.733%
53	14.642	2089	2092	2097	rVB	99707	101732	1.49%	0.251%
54	14.707	2101	2103	2108	rVB	225351	214488	3.14%	0.530%
55	14.960	2143	2146	2150	rVB	122137	122236	1.79%	0.302%
56	15.265	2194	2198	2202	rVV	748984	884908	12.97%	2.187%
57	15.312	2203	2206	2212	rVB	166386	200529	2.94%	0.496%
58	15.718	2271	2275	2282	rVB	153078	215437	3.16%	0.533%
59	16.189	2352	2355	2361	rVB	101737	145077	2.13%	0.359%

Sum of corrected areas: 40456043

LSC Report - Integrated Chromatogram

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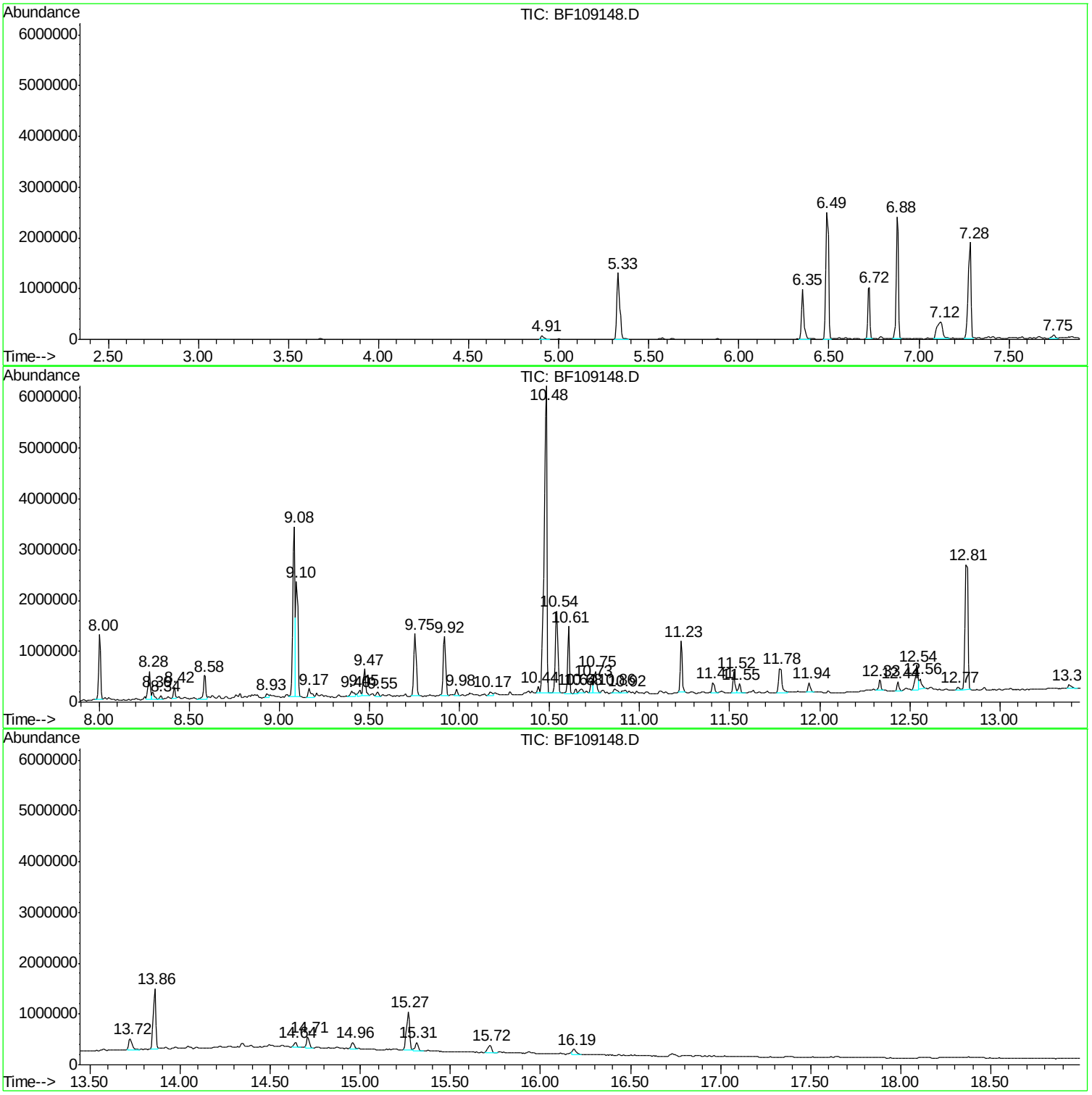
Data File : BF109148.D
Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109148.D
Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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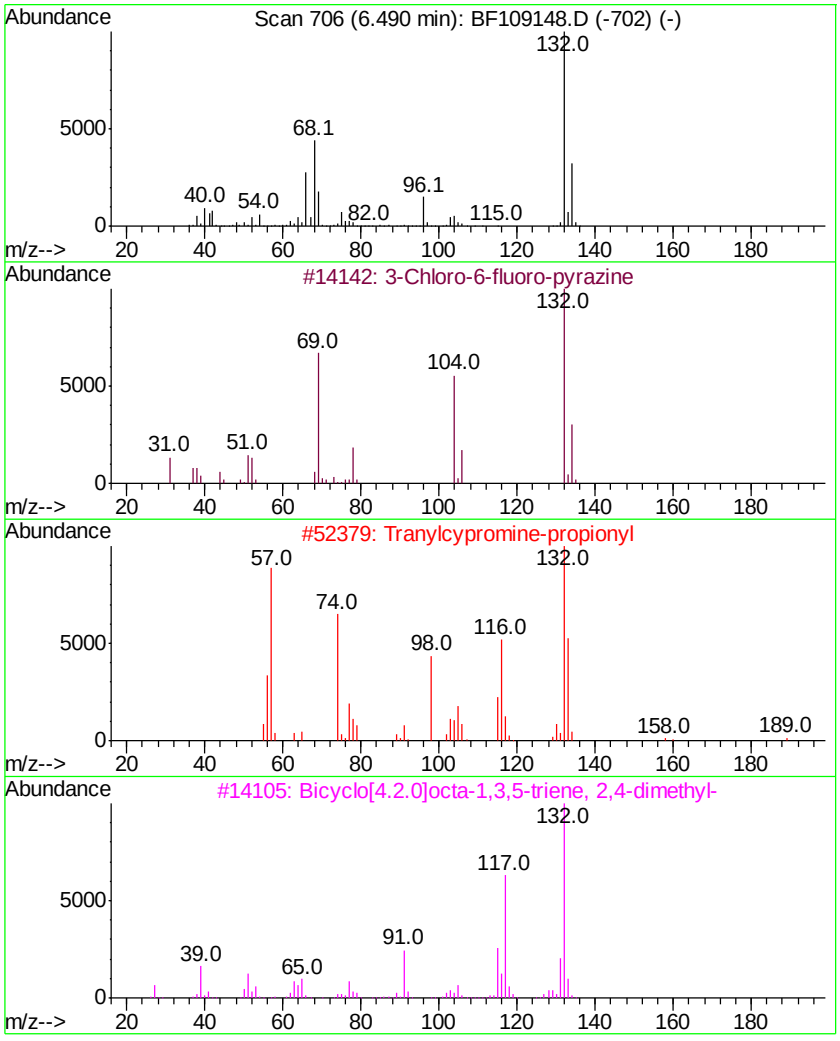
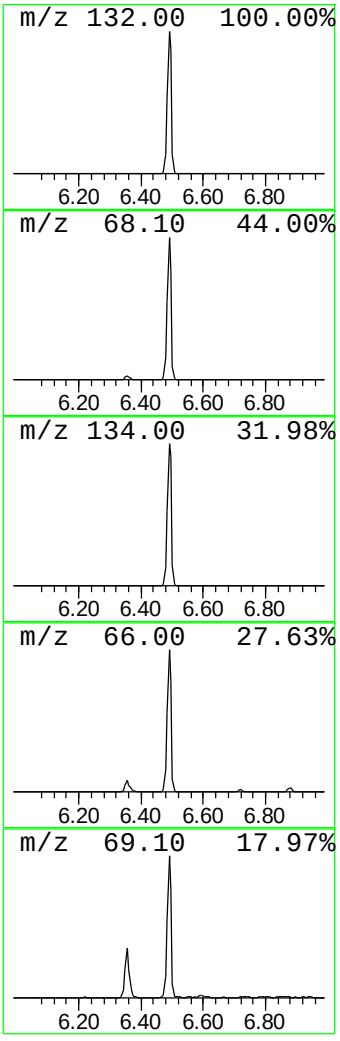
Peak Number 1 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	50.81 ng	2332490	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109148.D
Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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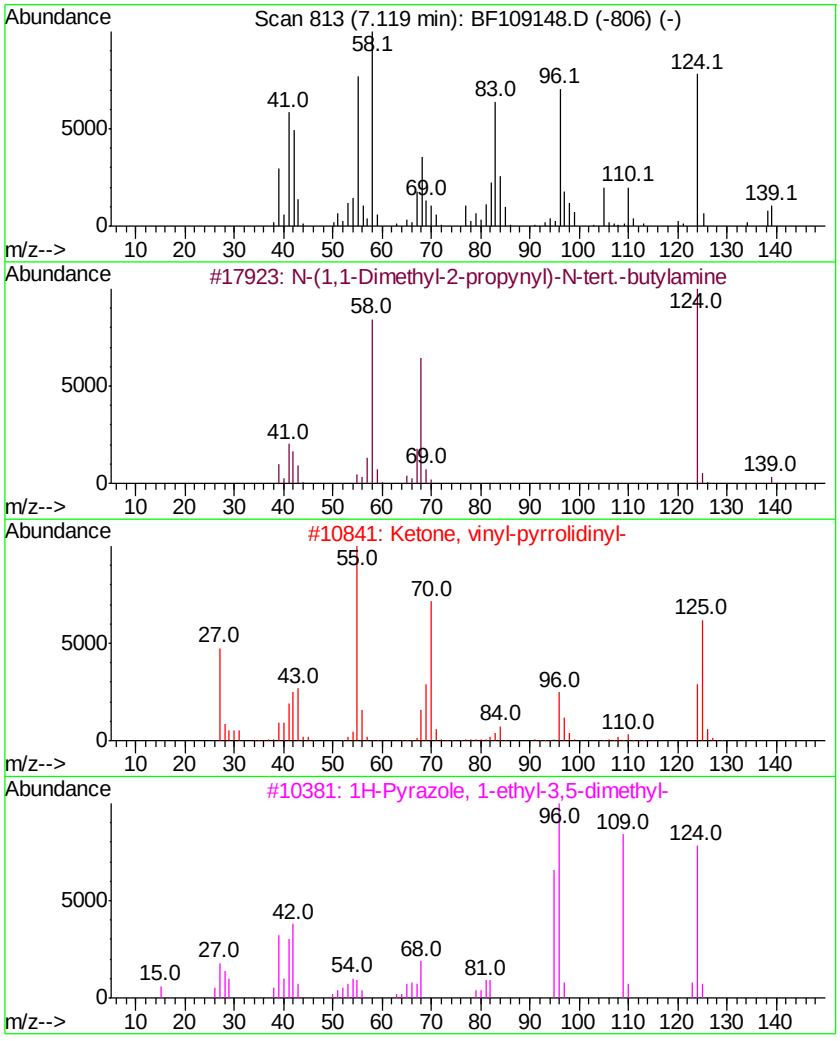
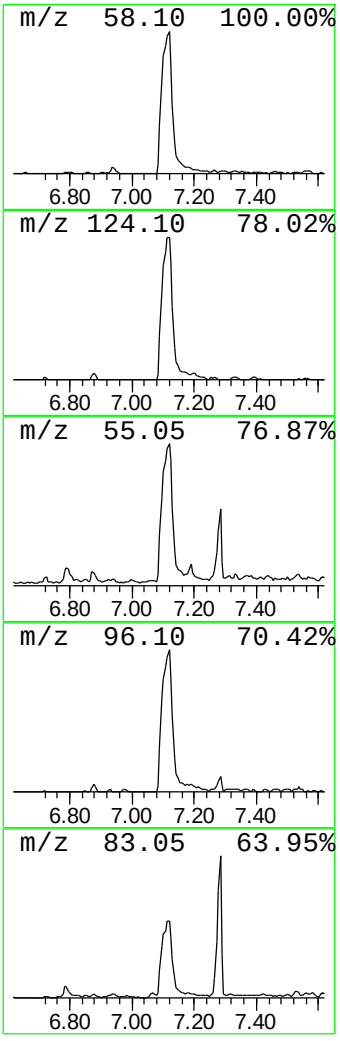
Peak Number 3 unknown7.12 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	16.04 ng	736133	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(1,1-Dimethyl-2-propynyl)-N-te...	139	C9H17N	001118-17-8	46
2	Ketone, vinyl-pyrrolidinyl-	125	C7H11NO	042104-70-1	38
3	1H-Pyrazole, 1-ethyl-3,5-dimethyl-	124	C7H12N2	017629-26-4	27
4	4,6-Dimethyl-2-pyrimidone	124	C6H8N2O	000108-79-2	27
5	1-Propenylaziridine	83	C5H9N	1000192-51-0	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
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Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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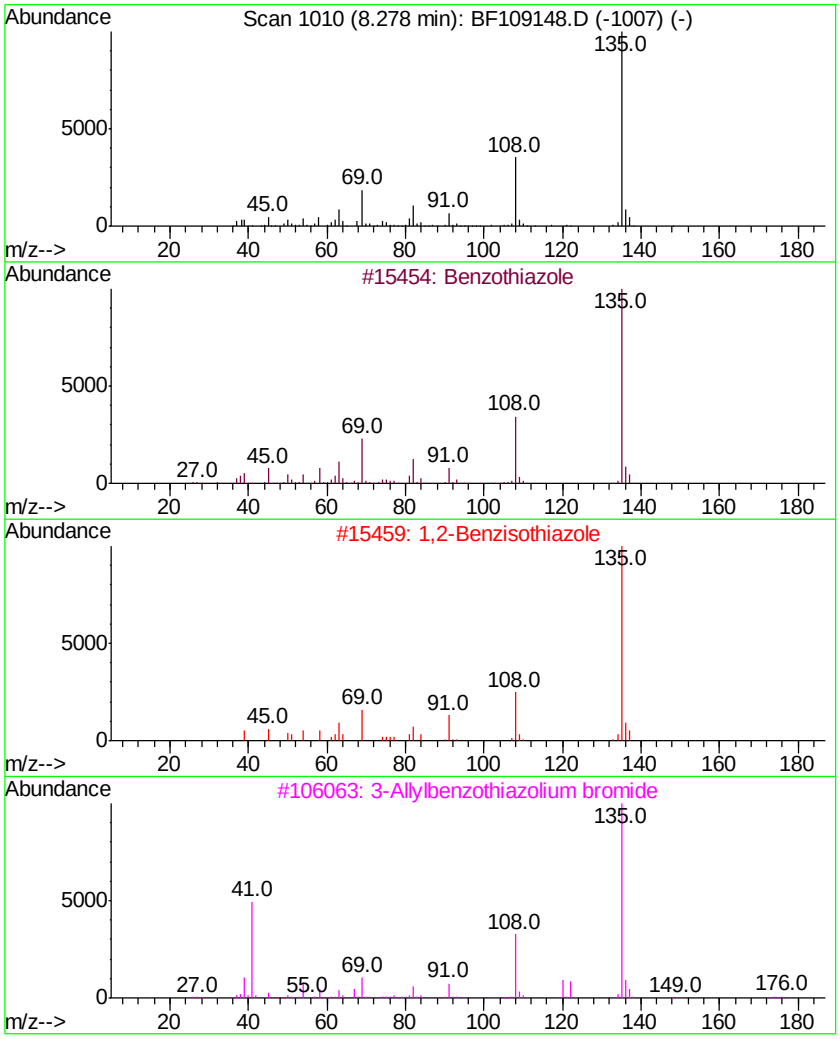
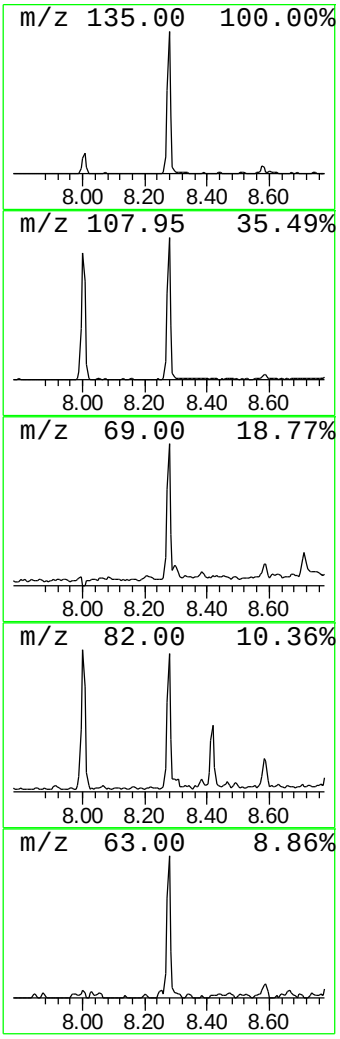
Peak Number 4 Benzothiazole Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	8.70 ng	467271	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	83
4	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	64
5	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
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Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

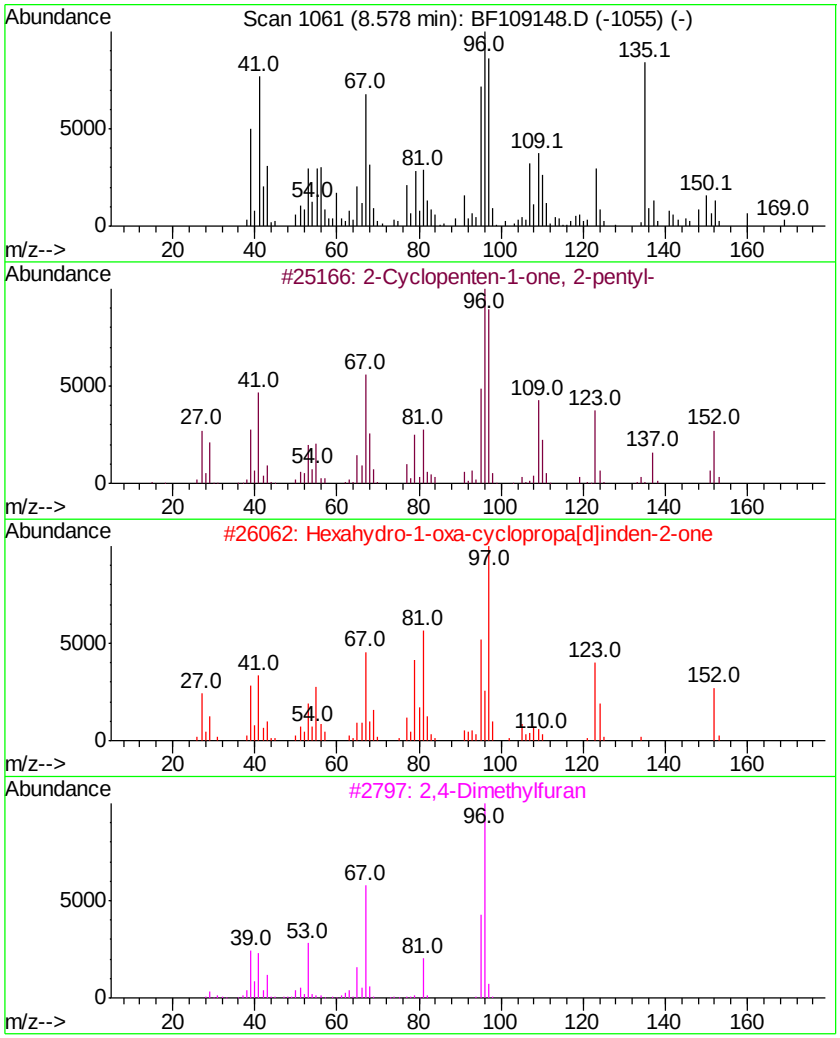
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

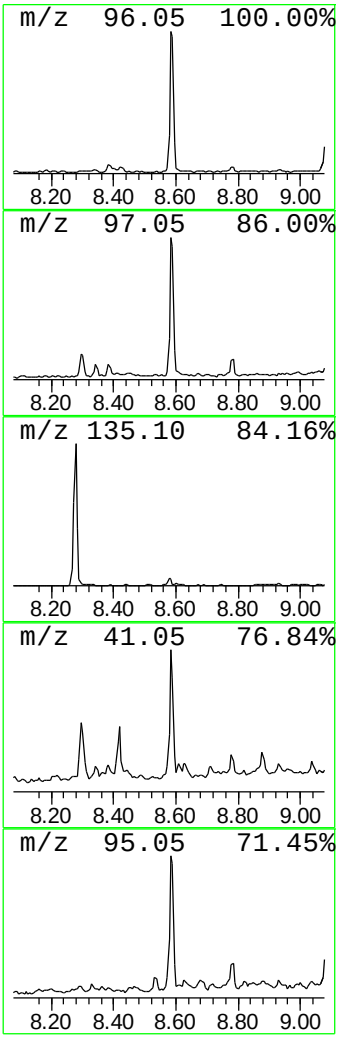
****

Peak Number 5 2-Cyclopenten-1-one, 2-pentyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.58	8.75 ng	469929	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 2-pentyl-	152	C10H16O	025564-22-1	96
2	Hexahydro-1-oxa-cyclopropa[d]ind...	152	C9H12O2	037643-23-5	38
3	2,4-Dimethylfuran	96	C6H8O	003710-43-8	38
4	Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	38
5	Spiro[4.4]nonane-1,6-dione	152	C9H12O2	027723-43-9	25





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : N48966

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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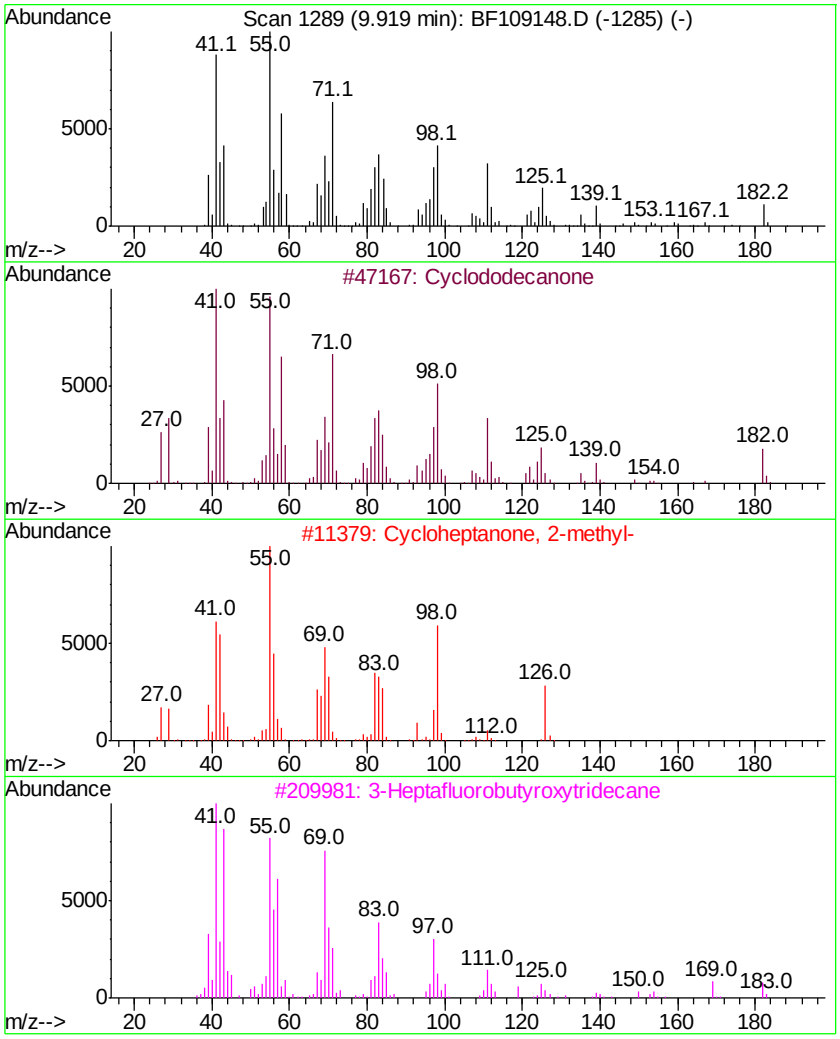
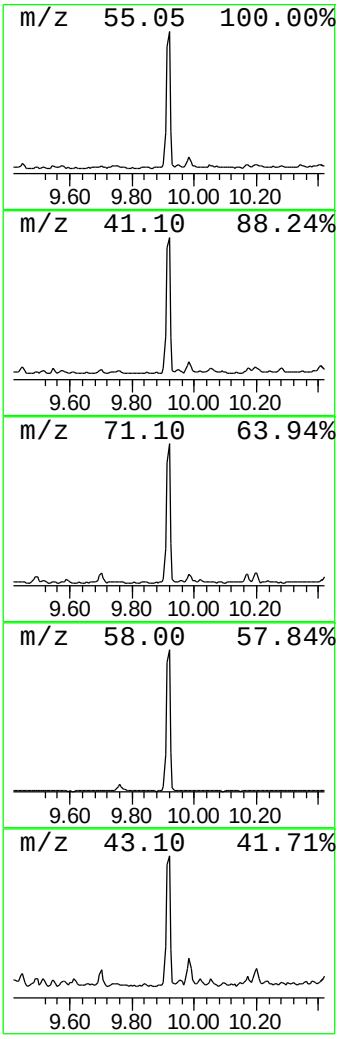
Peak Number 6 Cyclododecanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	19.04 ng	995538	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone	182	C12H22O	000830-13-7	98
2	Cycloheptanone, 2-methyl-	126	C8H14O	000932-56-9	35
3	3-Heptafluorobutyroxytridecane	396	C17H27F7O2	1000245-49-5	30
4	2-Tridecene, (E)-	182	C13H26	041446-58-6	25
5	2-Tridecene, (Z)-	182	C13H26	041446-59-7	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

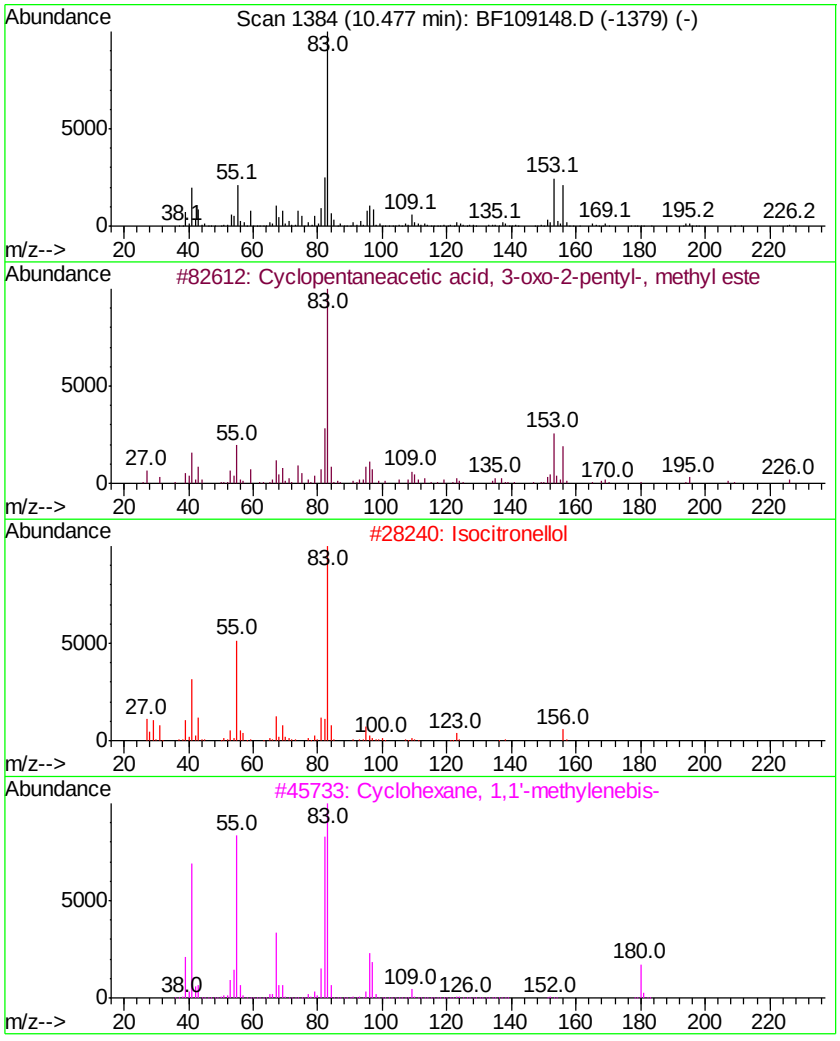
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

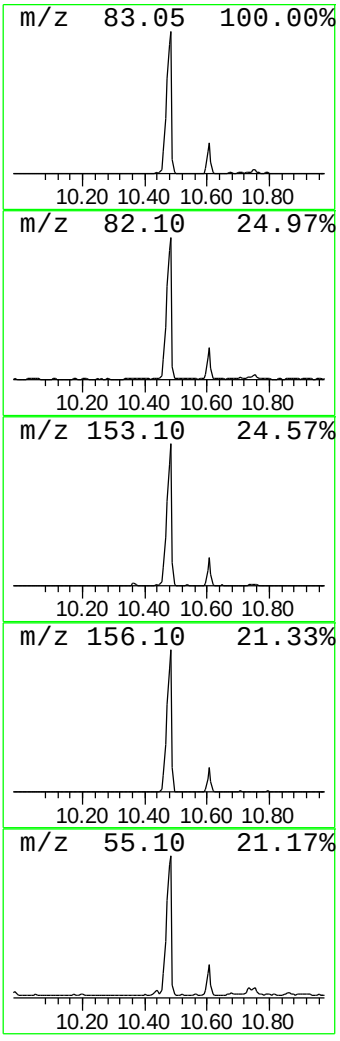
****

Peak Number 7 Cyclopentaneacetic acid, 3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.48	130.48 ng	6821280	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	90
2	Isocitronellol	156	C10H20O	018479-52-2	53
3	Cyclohexane, 1,1'-methylenebis-	180	C13H24	003178-23-2	43
4	Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	43
5	2-Nonen-4-one, 2-methyl-	154	C10H18O	002903-23-3	38





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Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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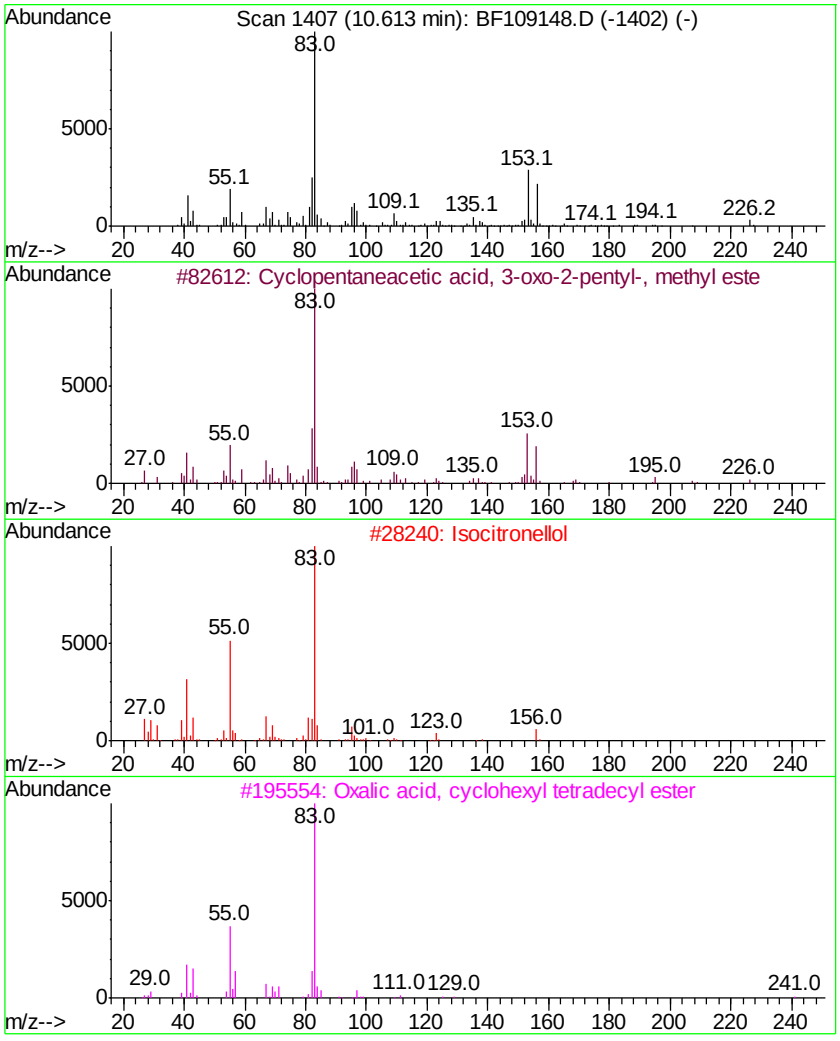
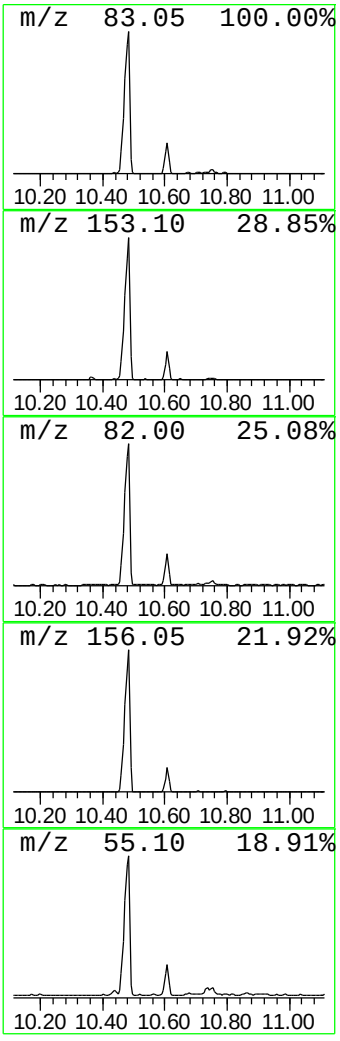
Peak Number 8 Isocitronellol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	24.34 ng	1019010	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	86
2	Isocitronellol	156	C10H20O	018479-52-2	50
3	Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	43
4	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	43
5	Cyclohexane, 1,1'-(1,2-ethanediy...	194	C14H26	003321-50-4	43





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Data File : BF109148.D
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Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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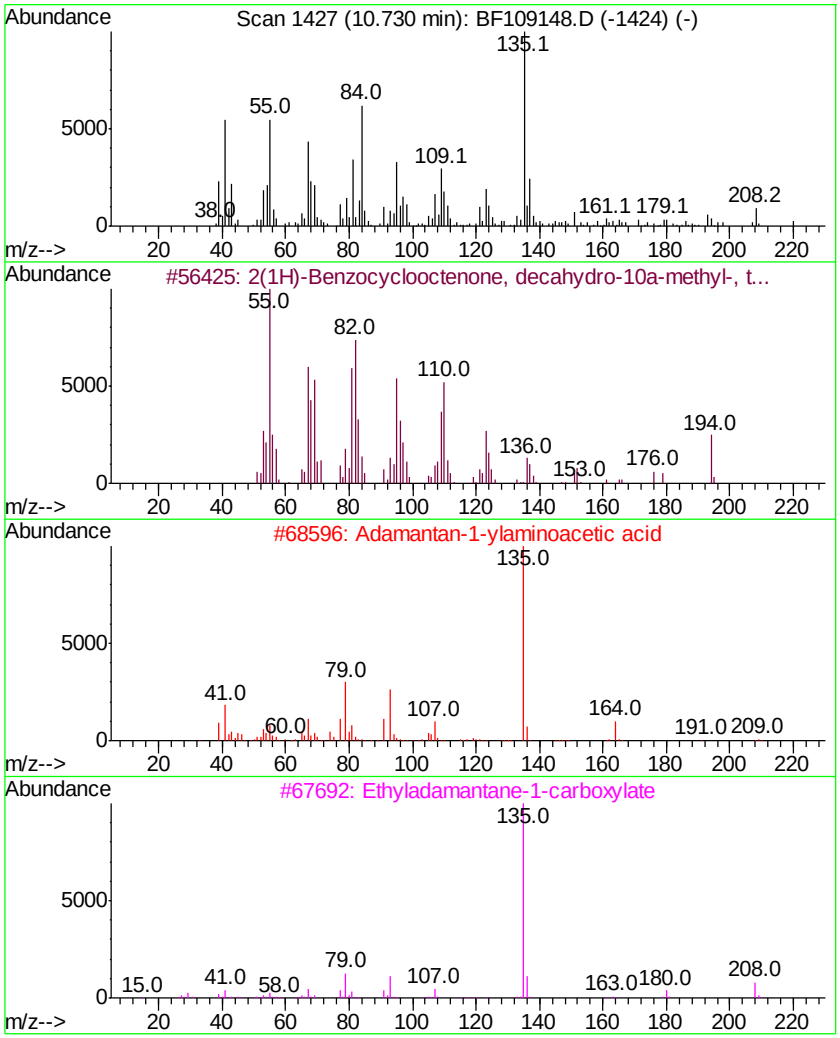
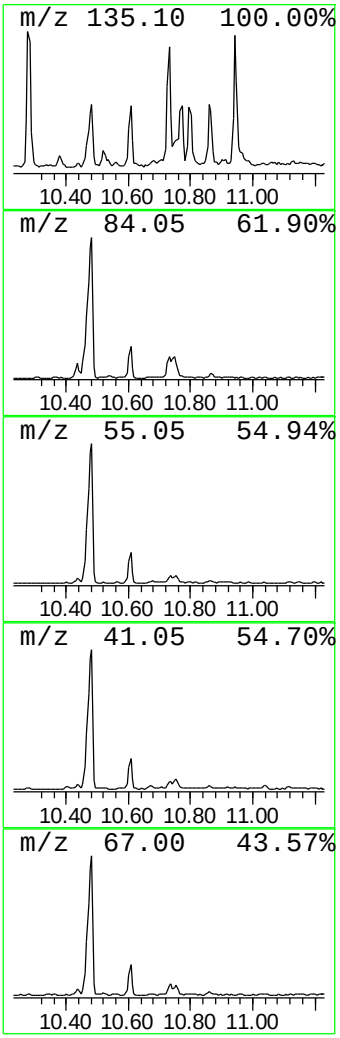
Peak Number 9 unknown10.73 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	6.17 ng	258183	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Benzocyclooctenone, decahy...	194	C13H22O	055103-68-9	27
2	Adamantan-1-ylaminoacetic acid	209	C12H19NO2	1000316-74-7	25
3	Ethyladamantane-1-carboxylate	208	C13H20O2	002094-73-7	25
4	3-(p-Methoxybenzoyl)-propionic acid	208	C11H12O4	003153-44-4	25
5	Tricyclo[3.3.1.1(3,7)]decane, 1-...	181	C10H15NO2	007575-82-8	22





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Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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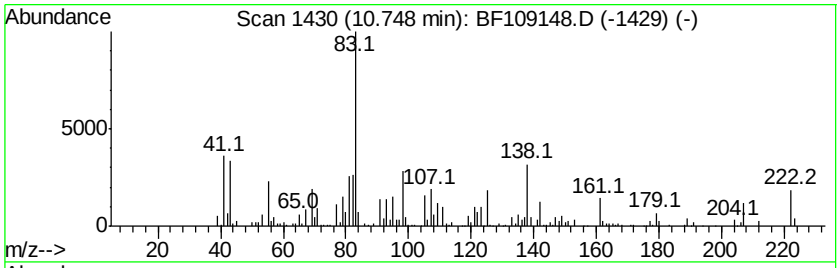
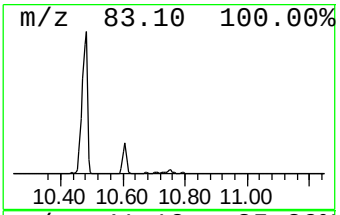
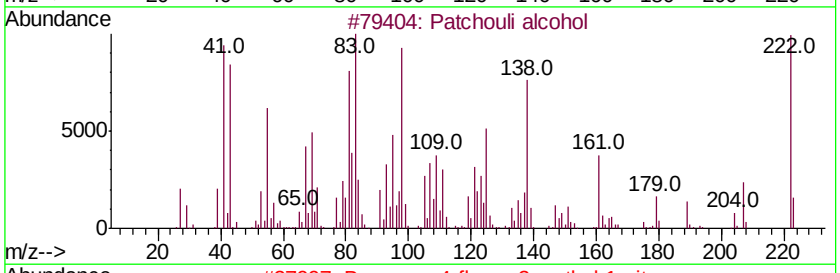
Peak Number 10 Patchouli alcohol Concentration Rank 9

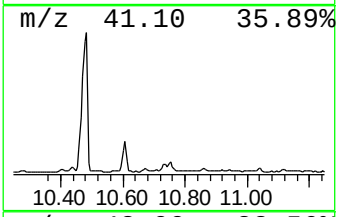
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	8.98 ng	376143	Phenanthrene-d10	11.23

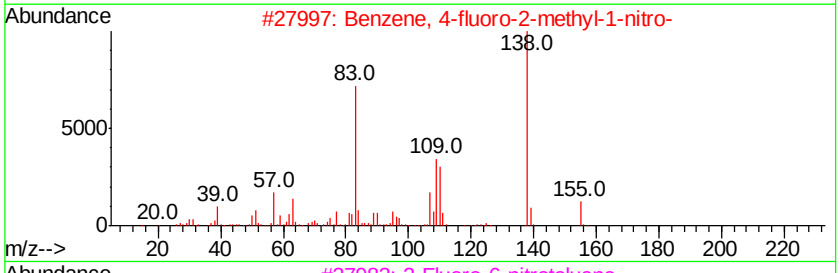
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Patchouli alcohol	222	C15H26O	005986-55-0	91
2	Benzene, 4-fluoro-2-methyl-1-nitro-	155	C7H6FNO2	000446-33-3	35
3	2-Fluoro-6-nitrotoluene	155	C7H6FNO2	000769-10-8	25
4	2H-Pyran, 3,4-dihydro-4-methyl-	98	C6H10O	002270-61-3	22
5	3-Decen-5-one	154	C10H18O	032064-73-6	16

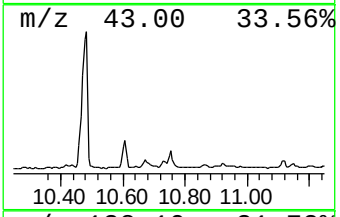


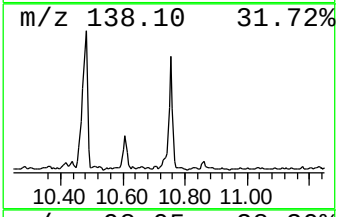


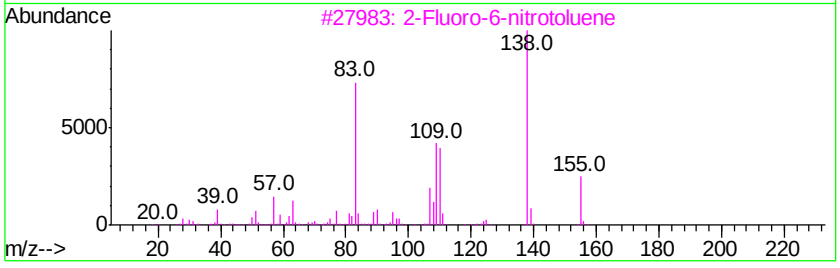


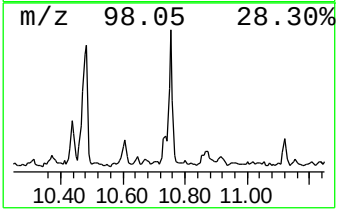












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Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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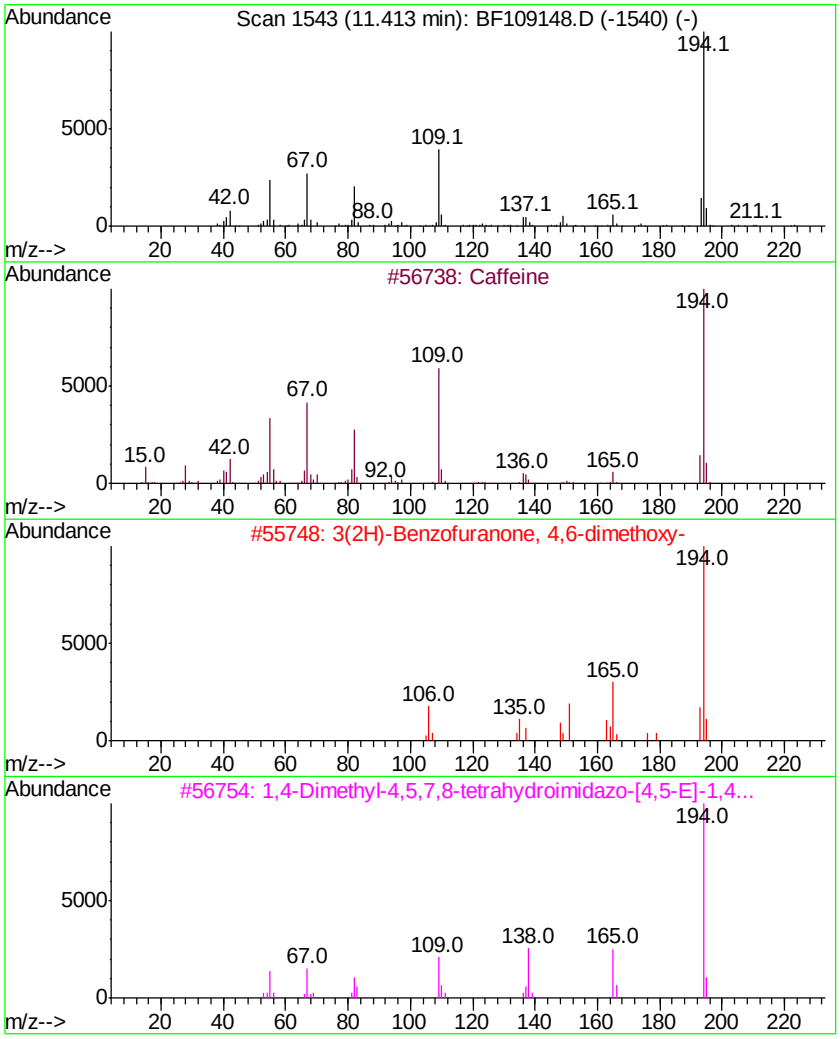
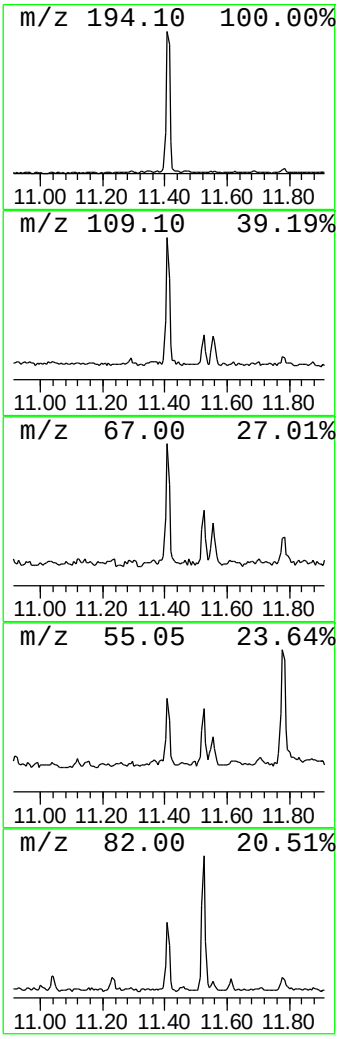
Peak Number 11 Caffeine Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	3.86 ng	161646	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	98
2	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	53
3	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	50
4	7-(Methylthio)pyrimido[4,5-d]pyr...	194	C7H6N4OS	091996-86-0	43
5	2H-Pyrazol-3-ol, 5-(2,5-dimethyl...	194	C9H10N2OS	1000304-22-5	43





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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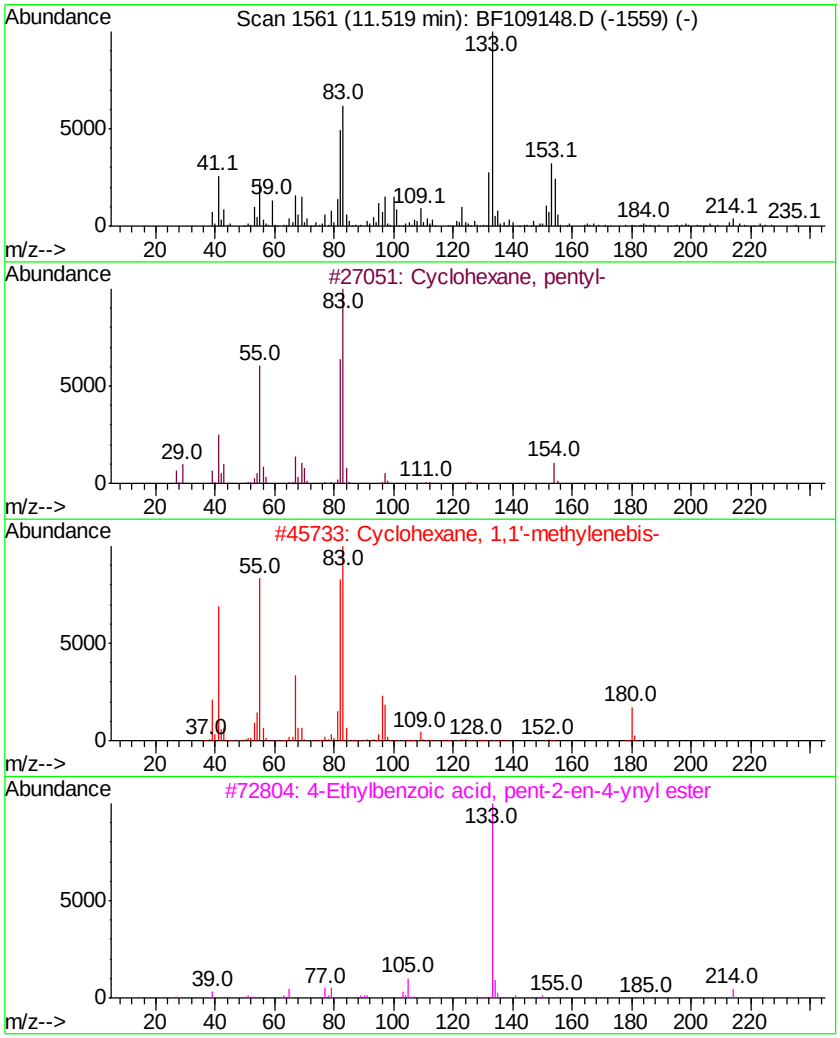
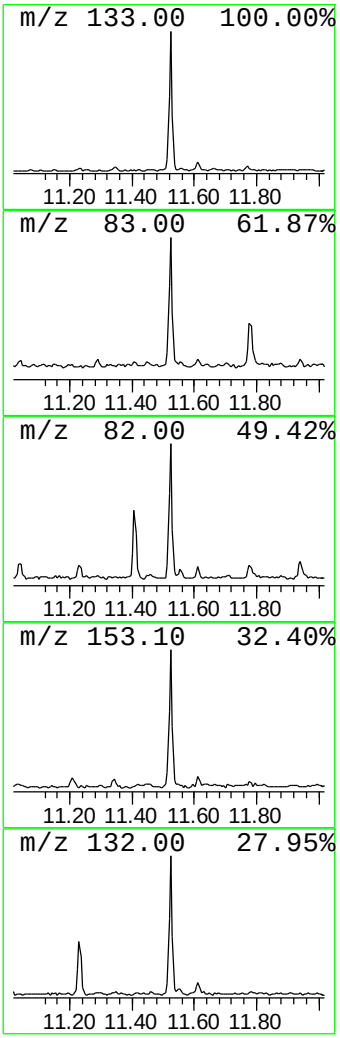
Peak Number 12 unknown11.52 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	7.72 ng	323397	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	27
2	Cyclohexane, 1,1'-methylenebis-	180	C13H24	003178-23-2	22
3	4-Ethylbenzoic acid, pent-2-en-4...	214	C14H14O2	1000292-54-2	18
4	Butyl glycolate, bromomethyldime...	282	C9H19BrO3Si	1000375-99-9	16
5	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	14





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Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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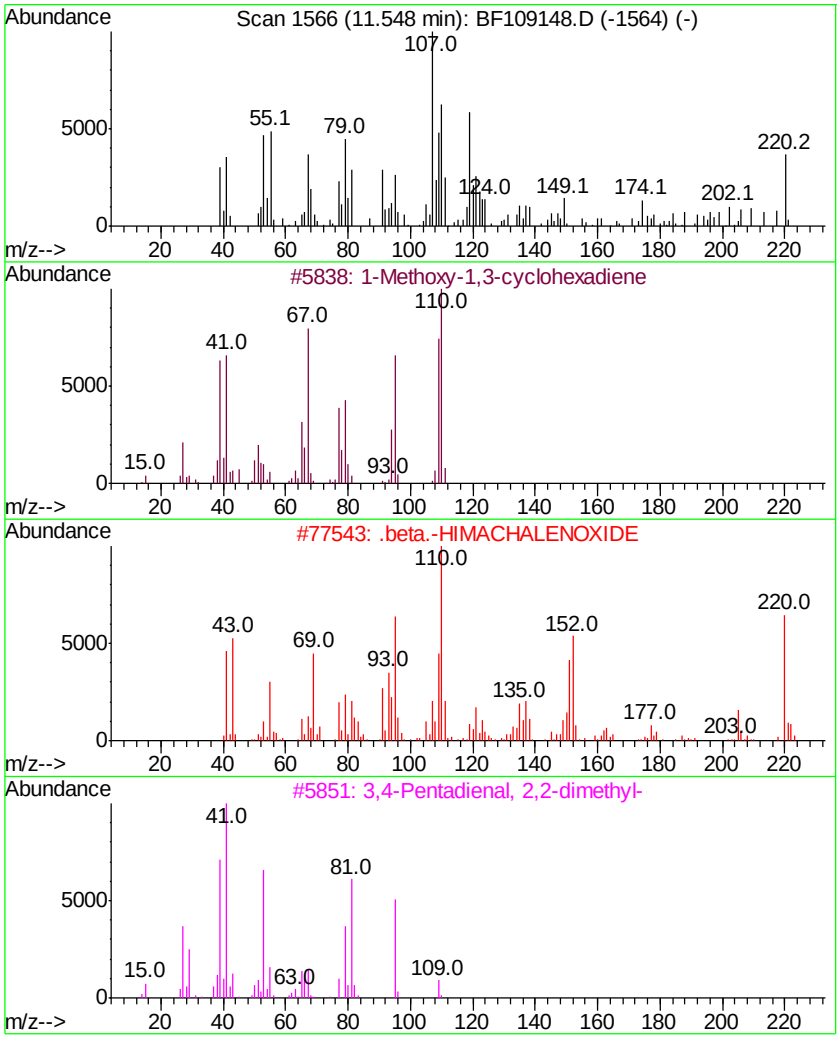
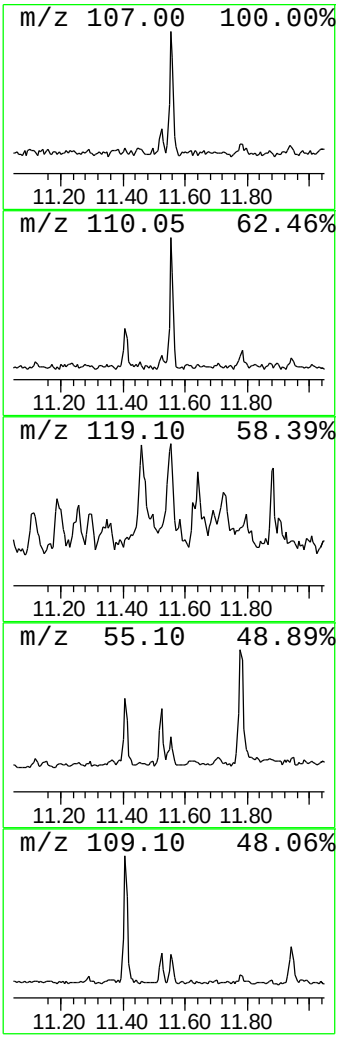
Peak Number 13 unknown11.55 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	4.24 ng	177647	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methoxy-1,3-cyclohexadiene	110	C7H10O	002161-90-2	35
2	.beta.-HIMACHALENOXIDE	220	C15H24O	1000140-21-6	18
3	3,4-Pentadienal, 2,2-dimethyl-	110	C7H10O	004058-51-9	16
4	1,3-Cyclopentadiene, 2-bromo-3-(...	182	C8H7Br	1000142-00-7	14
5	2-Cyclohexen-1-one dimethylketal	142	C8H14O2	001728-18-3	14





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Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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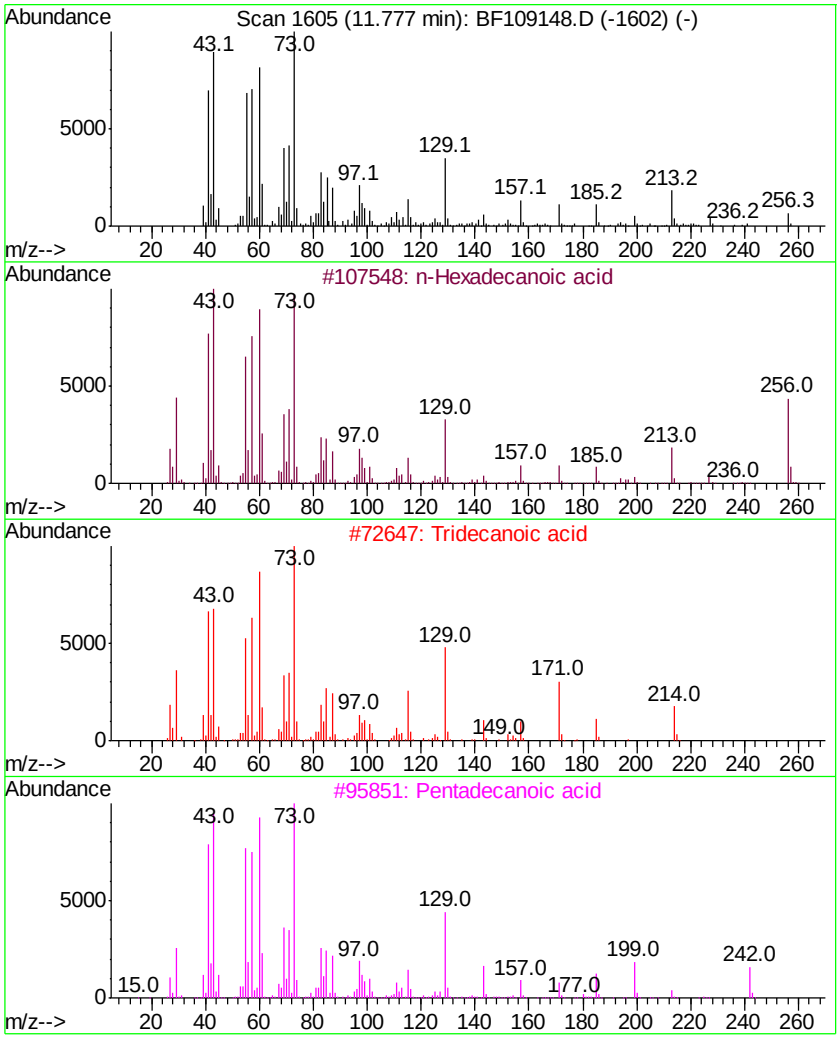
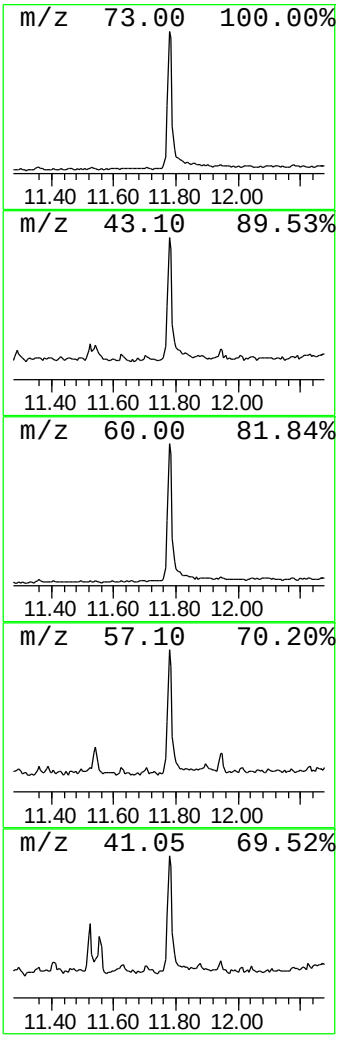
Peak Number 14 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	12.90 ng	539954	Phenanthrene-d10	11.23

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





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Instrument : BNA_F
ClientSampleId : N48966

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TIC Library : C:\DATABASE\NIST11.L
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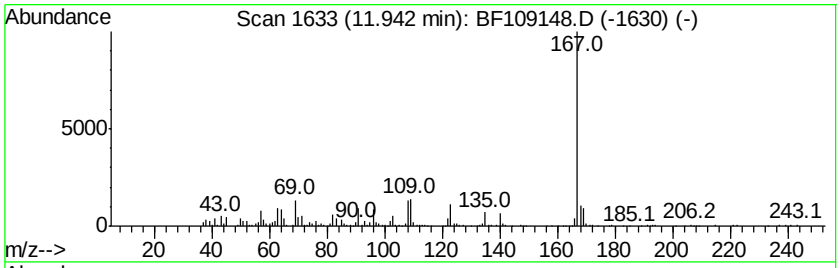
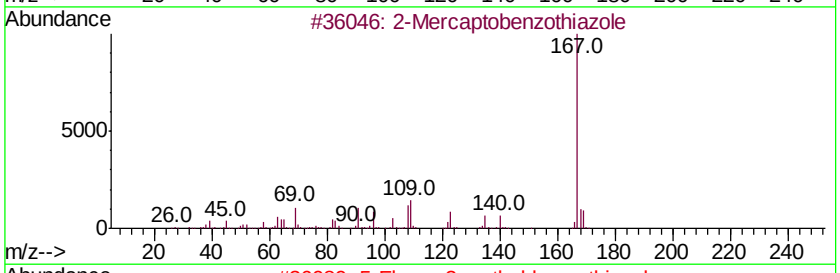
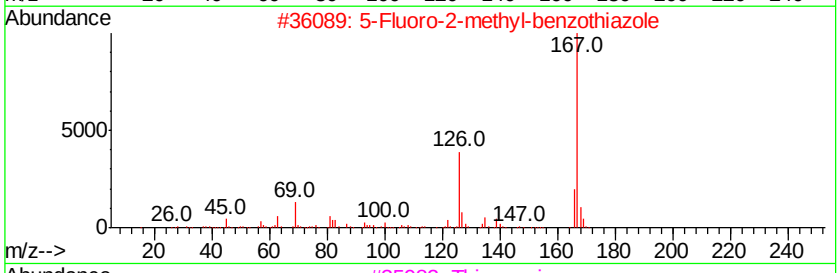
Peak Number 15 2-Mercaptobenzothiazole Concentration Rank 19

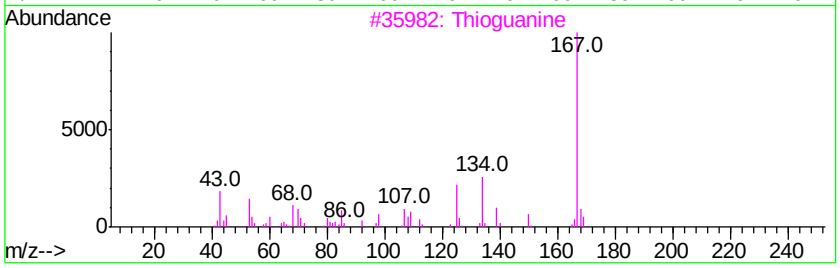
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	4.16 ng	174035	Phenanthrene-d10	11.23

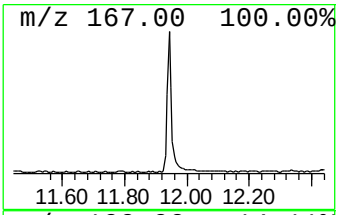
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	59
3	Thioguanine	167	C5H5N5S	000154-42-7	59
4	Mandelic acid, 3,4-dimethoxy-, m...	226	C11H14O5	002911-73-1	56
5	Benzothiazole, 2-(2-hydroxyethyl...	211	C9H9NOS2	004665-63-8	56

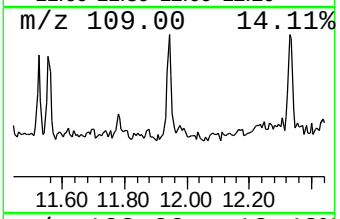


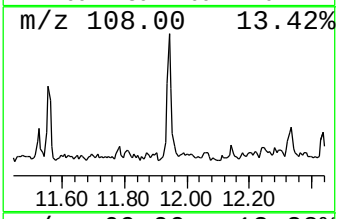


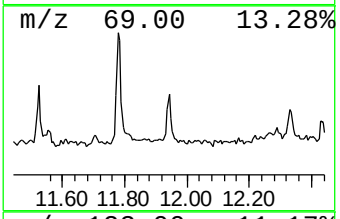


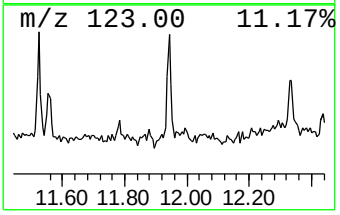












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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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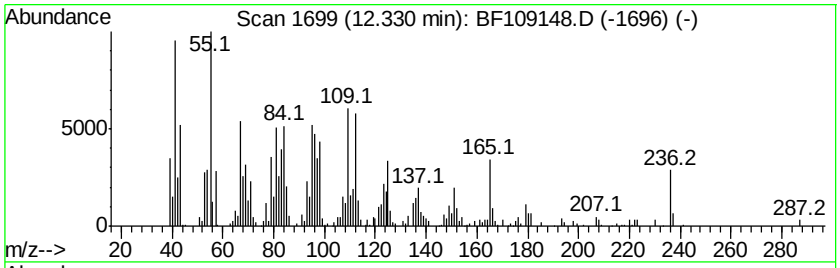
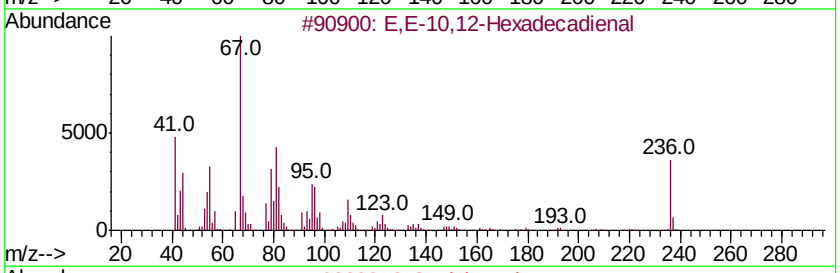
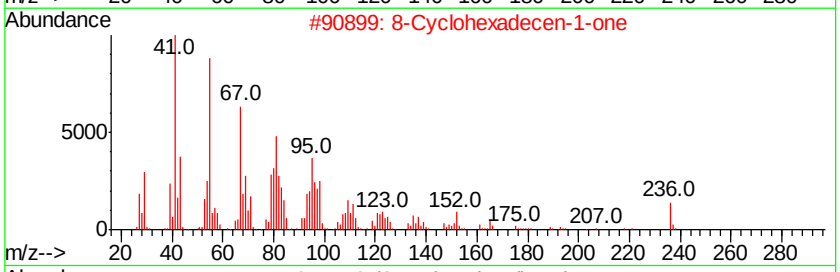
Peak Number 16 E,E-10,12-Hexadecadienal Concentration Rank 18

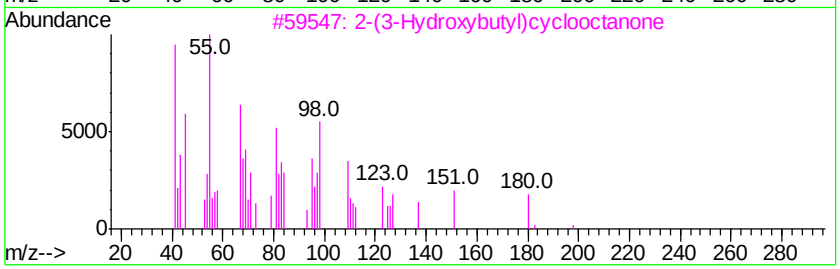
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	4.18 ng	175215	Phenanthrene-d10	11.23

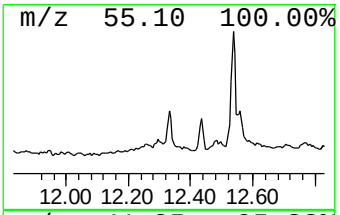
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E,E-10,12-Hexadecadienal	236	C16H28O	1000130-85-8	74
2	8-Cyclohexadecen-1-one	236	C16H28O	003100-36-5	43
3	2-(3-Hydroxybutyl)cyclooctanone	198	C12H22O2	110288-21-6	38
4	4-Cyclohexylidene-n-butanol	154	C10H18O	004441-58-1	25
5	2,2,6,7-Tetramethyl-10-oxatricyc...	208	C13H20O2	121747-63-5	25

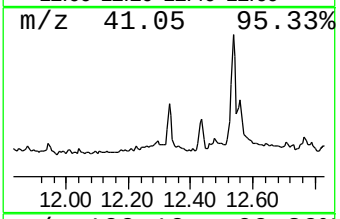


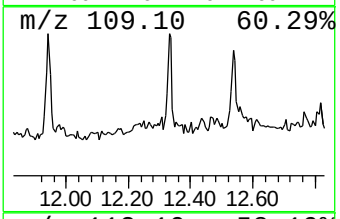


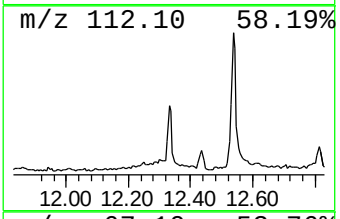


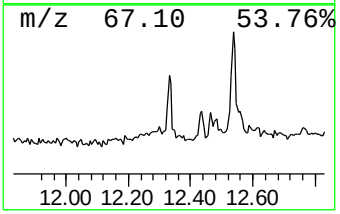












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109148.D
Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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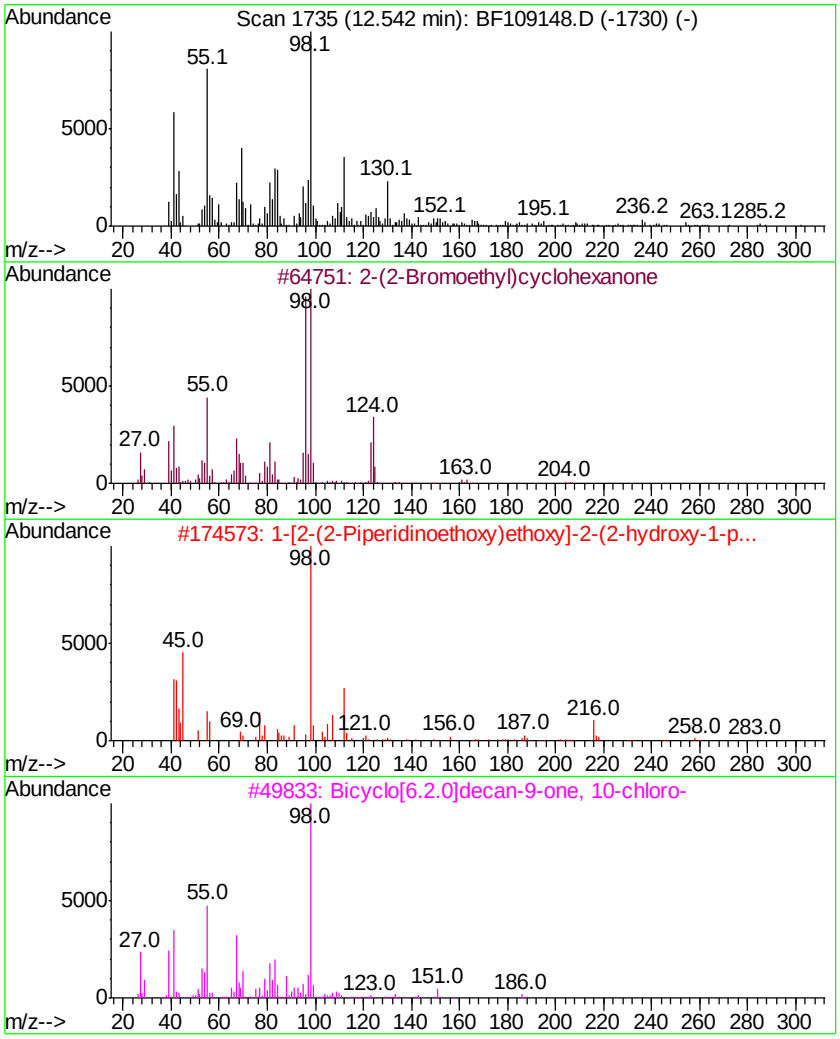
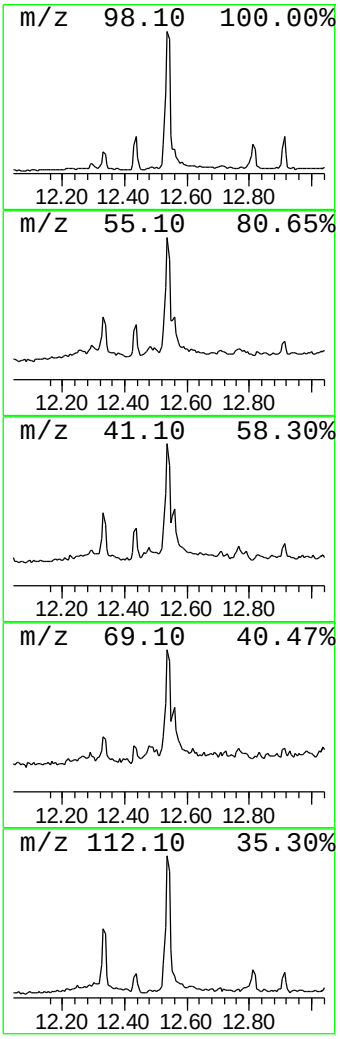
Peak Number 17 unknown12.54 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	12.49 ng	523104	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Bromoethyl)cyclohexanone	204	C8H13BrO	1000195-45-9	49
2	1-[2-(2-Piperidinoethoxy)ethoxy]...	337	C19H31NO4	1000215-99-3	38
3	Bicyclo[6.2.0]decan-9-one, 10-ch...	186	C10H15ClO	1000152-62-7	38
4	Aziridine, 2-methyl-3-(1-methyle...	139	C9H17N	055669-77-7	35
5	3H-Pyrazol-3-one, 1,2-dihydro-5-...	98	C4H6N2O	004344-87-0	35





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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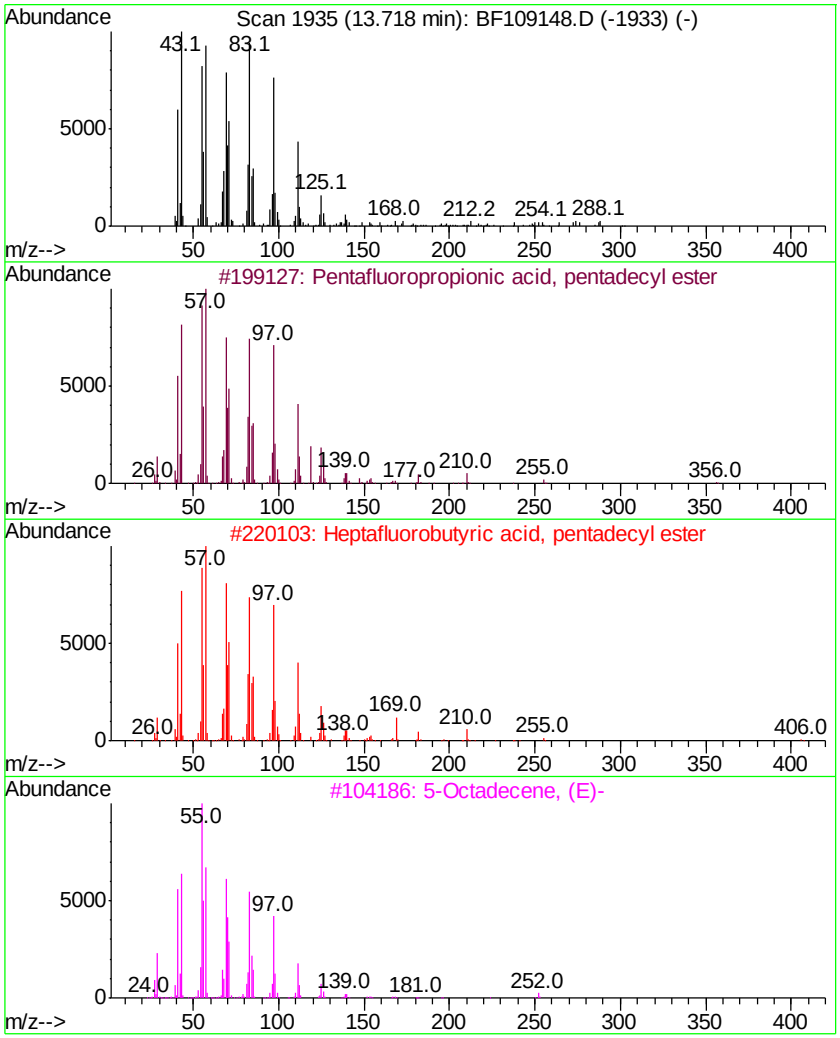
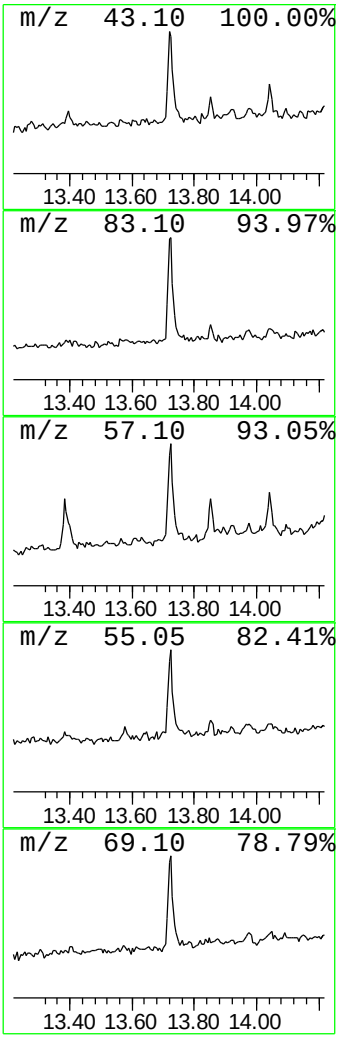
Peak Number 18 Pentafluoropropionic acid, ... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.54 ng	250967	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	93





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Sample : J4957-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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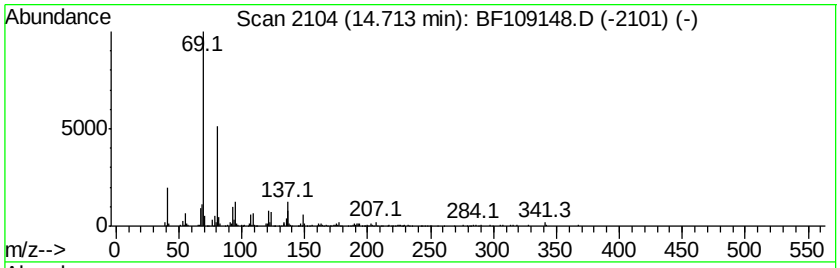
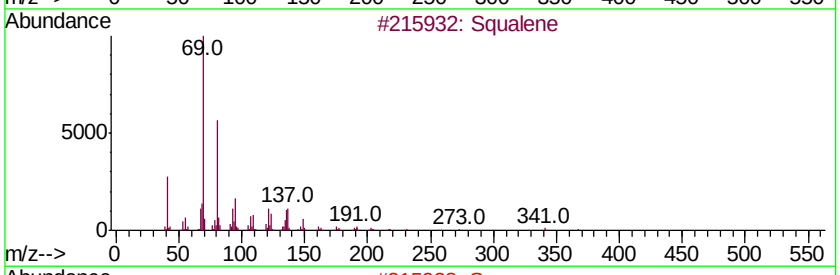
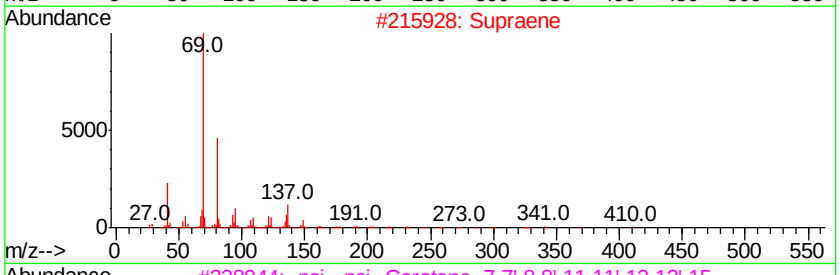
Peak Number 19 Squalene Concentration Rank 15

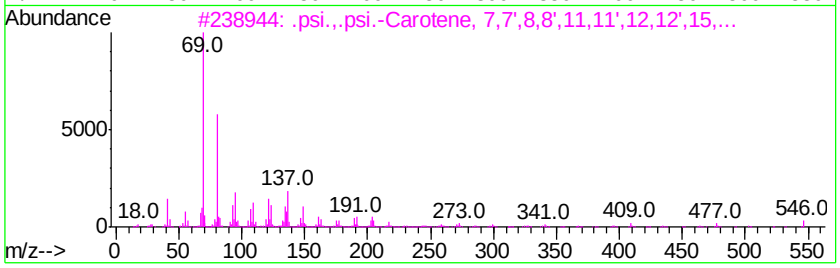
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	4.85 ng	214488	Perylene-d12	15.27

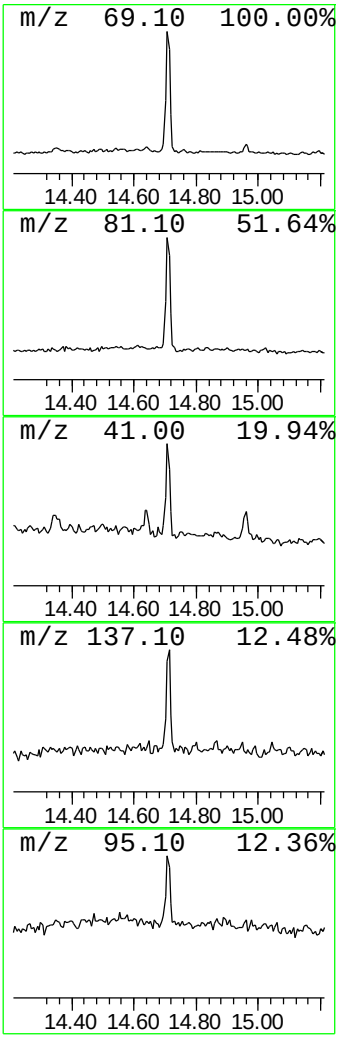
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	1,3,5-Tris(cyanomethyl)-S-hexahy...	204	C9H12N6	004560-87-6	50











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Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
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Instrument : BNA_F
ClientSampleId : N48966

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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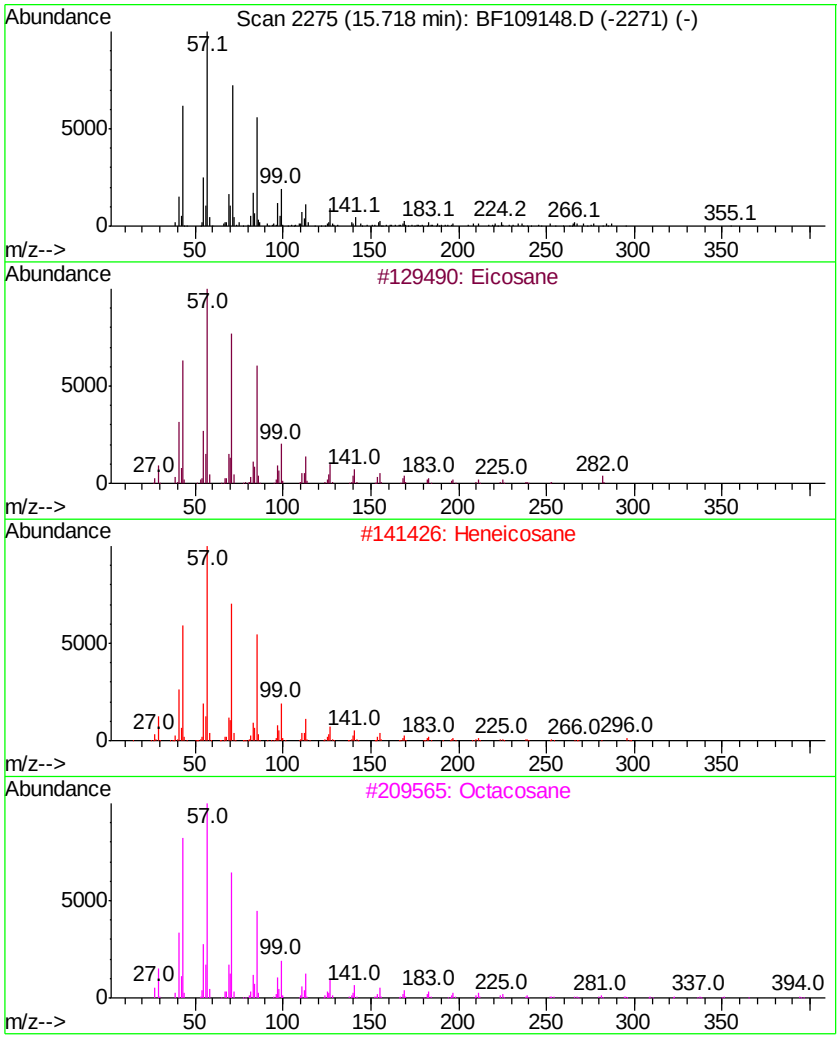
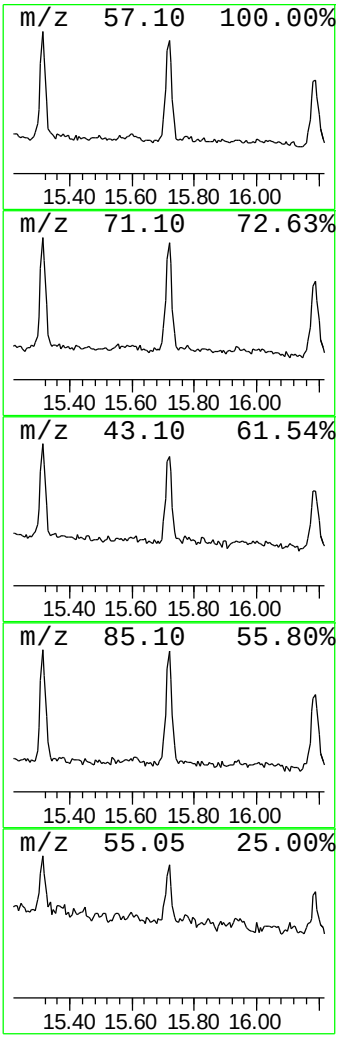
Peak Number 20 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.87 ng	215437	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptacosane	380	C27H56	000593-49-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091918\
Data File : BF109148.D
Acq On : 19 Sep 2018 17:22
Operator : JU/SJ
Sample : J4957-01
Misc :
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Instrument : BNA_F
ClientSampleId : N48966

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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
unknown6.49	6.49	50.8	ng	2332490	1	6.72	918082	20.0
unknown7.12	7.12	16.0	ng	736133	1	6.72	918082	20.0
Benzothiazole	8.28	8.7	ng	467271	2	8.00	1073720	20.0
2-Cyclopenten-1-o...	8.58	8.8	ng	469929	2	8.00	1073720	20.0
Cyclododecanone	9.92	19.0	ng	995538	3	9.75	1045550	20.0
Cyclopentaneaceti...	10.48	130.5	ng	6821280	3	9.75	1045550	20.0
Isocitronellol	10.61	24.3	ng	1019010	4	11.23	837389	20.0
unknown10.73	10.73	6.2	ng	258183	4	11.23	837389	20.0
Patchouli alcohol	10.75	9.0	ng	376143	4	11.23	837389	20.0
Caffeine	11.41	3.9	ng	161646	4	11.23	837389	20.0
unknown11.52	11.52	7.7	ng	323397	4	11.23	837389	20.0
unknown11.55	11.55	4.2	ng	177647	4	11.23	837389	20.0
n-Hexadecanoic acid	11.78	12.9	ng	539954	4	11.23	837389	20.0
2-Mercaptobenzoth...	11.94	4.2	ng	174035	4	11.23	837389	20.0
E,E-10,12-Hexadec...	12.33	4.2	ng	175215	4	11.23	837389	20.0
unknown12.54	12.54	12.5	ng	523104	4	11.23	837389	20.0
Pentafluoropropio...	13.72	4.5	ng	250967	5	13.86	1105490	20.0
Squalene	14.71	4.8	ng	214488	6	15.27	884908	20.0
Eicosane	15.72	4.9	ng	215437	6	15.27	884908	20.0