LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090828.D
Acq On : 26 Oct 2016 00:43
Operator : UM/SJ
Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

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-BF102116.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	4.967	249	252	259	rBV	438940	613050	15.84%	1.702%
2	5.390	287	289	292	rBV	2155677	2767990	71.53%	7.684%
3	6.442	378	381	383	rBV	2950340	3426932	88.56%	9.514%
4	6.567	389	392	394	rBV	3537847	3544520	91.60%	9.840%
5	6.796	410	412	423	rBV	1069694	1071700	27.70%	2.975%
6	6.956	423	426	428	rBV	2726793	2659479	68.73%	7.383%
7	7.367	459	462	464	rBV	1640163	1812231	46.83%	5.031%
8	7.470	469	471	477	rVB	49824	82620	2.14%	0.229%
9	8.087	522	525	527	rBV	1400863	1340549	34.64%	3.722%
10	9.162	617	619	622	rBV	3876665	3869637	100.00%	10.743%
11	9.562	651	654	656	rBV	1100694	913176	23.60%	2.535%
12	9.836	676	678	681	rBV	1651339	1593349	41.18%	4.423%
13	10.282	715	717	718	rVB	66536	57614	1.49%	0.160%
14	10.499	733	736	739	rBV	28979	43542	1.13%	0.121%
15	10.625	745	747	750	rBV2	1847708	2167494	56.01%	6.017%
16	10.751	756	758	765	rVB	105843	139009	3.59%	0.386%
17	11.196	796	797	799	rBV2	49862	51001	1.32%	0.142%
18	11.322	806	808	812	rBV	1471301	1314518	33.97%	3.649%
19	12.796	933	937	945	rBV	613886	854536	22.08%	2.372%
20	12.911	945	947	950	rBV	3512034	3276217	84.66%	9.095%
21	13.128	964	966	970	rVB2	31357	61447	1.59%	0.171%
22	13.814	1023	1026	1030	rBV	298302	344840	8.91%	0.957%
23	13.962	1036	1039	1041	rBV	921411	959720	24.80%	2.664%
24	14.145	1053	1055	1058	rBV2	21770	38726	1.00%	0.108%
25	14.454	1079	1082	1085	rBV	232941	362298	9.36%	1.006%
26	14.808	1111	1113	1116	rVB	48838	58166	1.50%	0.161%
27	14.877	1117	1119	1122	rVB	104921	113333	2.93%	0.315%
28	15.082	1133	1137	1141	rBV2	105850	260254	6.73%	0.723%
29	15.380	1160	1163	1166	rBV	712120	888293	22.96%	2.466%
30	15.608	1181	1183	1187	rVB	61648	85346	2.21%	0.237%
31	15.825	1200	1202	1205	rBV	64016	104537	2.70%	0.290%
32	15.883	1205	1207	1210	rBV3	33502	69474	1.80%	0.193%
33	15.940	1210	1212	1217	rVB2	24293	56502	1.46%	0.157%
34	16.340	1241	1247	1249	rBV4	18048	76584	1.98%	0.213%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090828.D
Acq On : 26 Oct 2016 00:43
Operator : UM/SJ
Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

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-BF102116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.568	1264	1267	1272	rVB	68748	131058	3.39%	0.364%
36	16.854	1289	1292	1294	rBV2	28872	58565	1.51%	0.163%
37	16.911	1294	1297	1303	rVV4	60791	162119	4.19%	0.450%
38	17.025	1304	1307	1309	rVV	28096	65632	1.70%	0.182%
39	17.071	1309	1311	1317	rVB4	32910	74464	1.92%	0.207%
40	17.300	1327	1331	1335	rBV5	33803	96342	2.49%	0.267%
41	17.906	1381	1384	1387	rBV3	27288	76359	1.97%	0.212%
42	18.260	1411	1415	1422	rBV7	22339	81732	2.11%	0.227%
43	19.220	1495	1499	1508	rVB5	56649	195961	5.06%	0.544%

Sum of corrected areas: 36020916

LSC Report - Integrated Chromatogram

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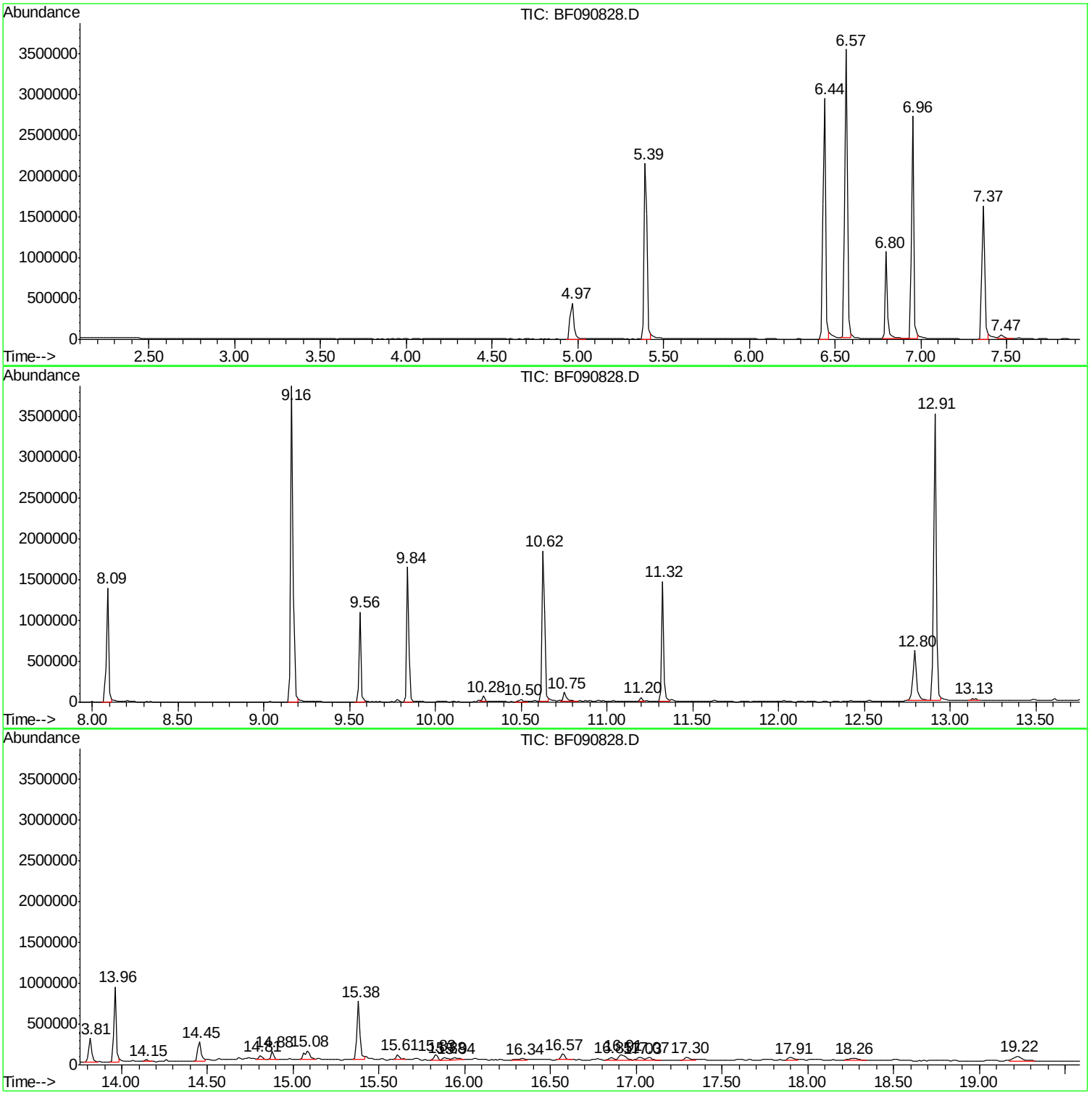
Operator : UM/SJ
Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090828.D
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Sample : H5396-07
Misc :
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Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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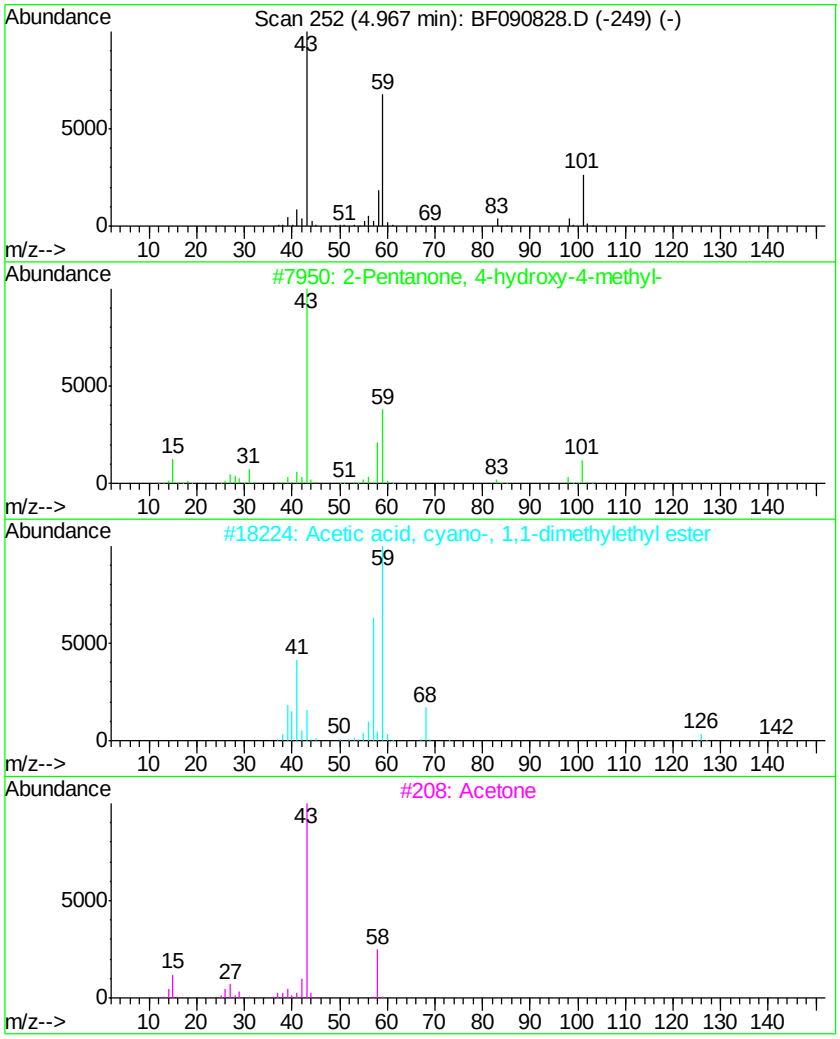
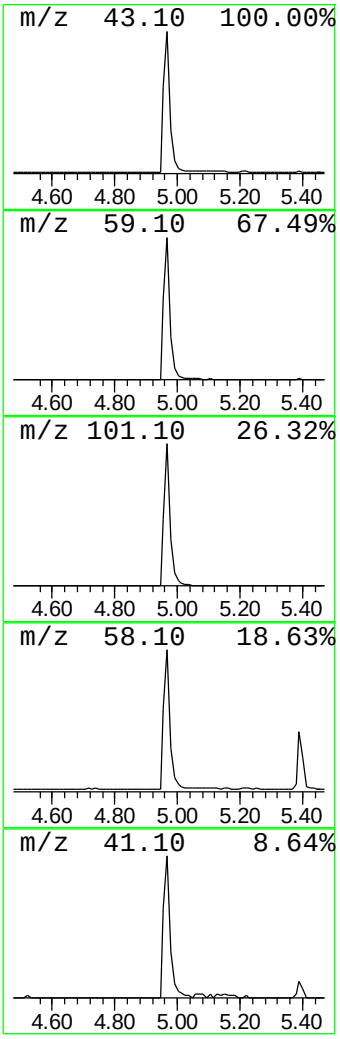
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	11.44 ng	613050	1,4-Dichlorobenzene-d4	6.80

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	17
3	Acetone	58	C3H6O	000067-64-1	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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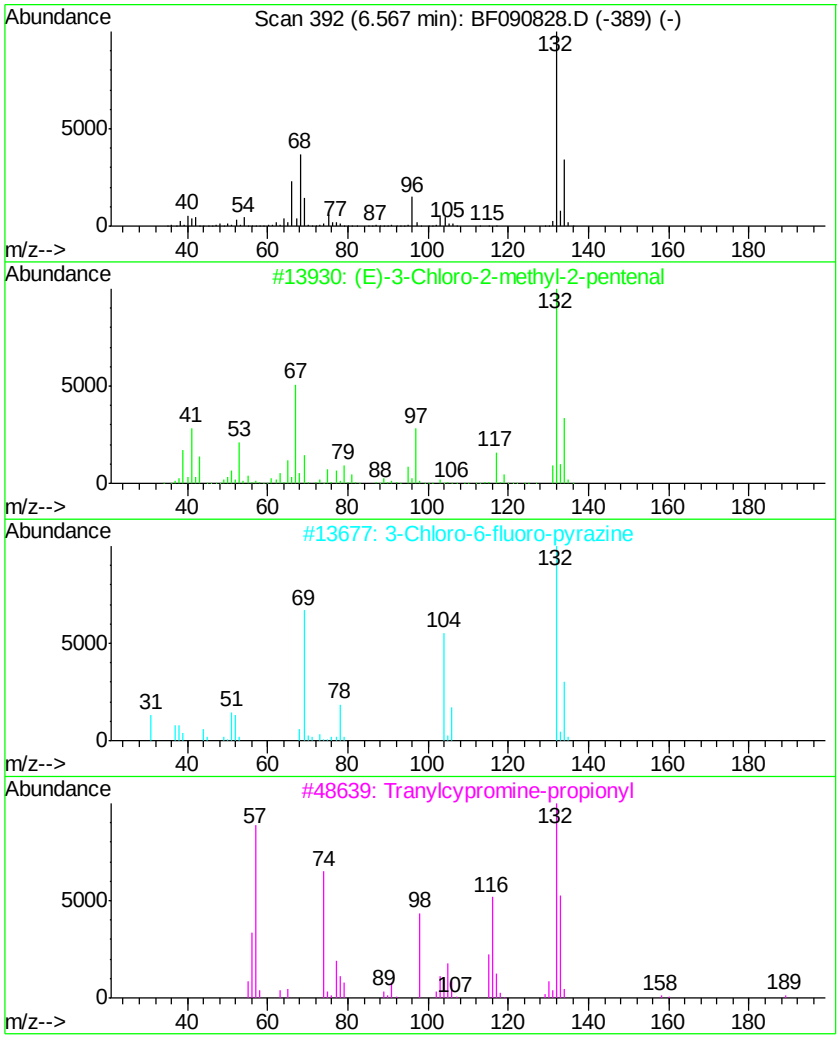
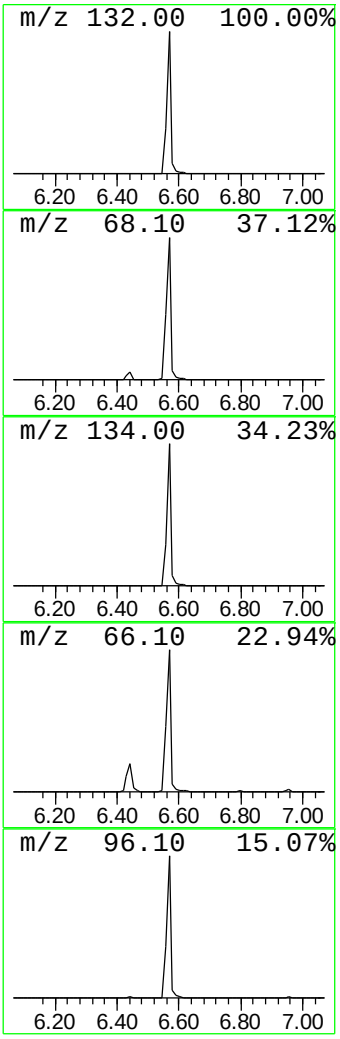
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	66.15 ng	3544520	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Operator : UM/SJ
Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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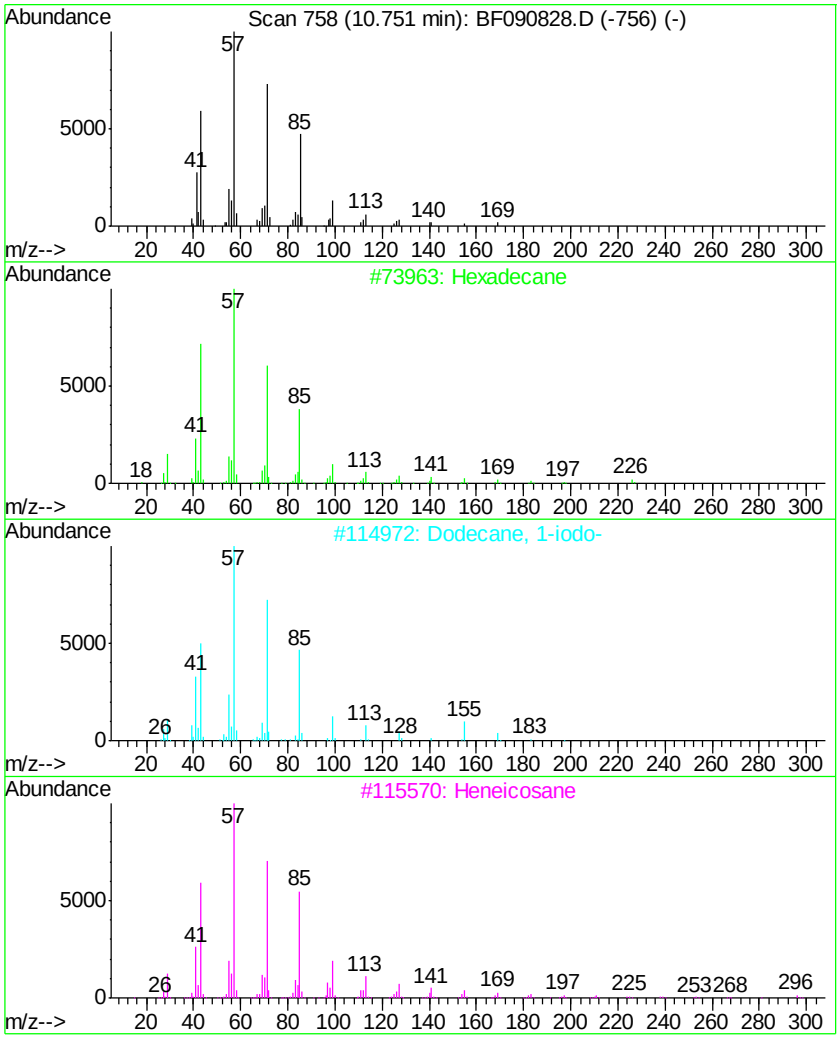
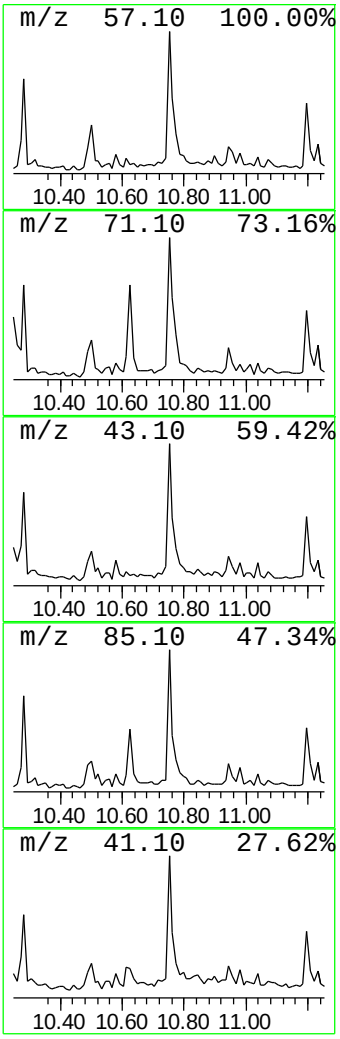
Peak Number 4 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.11 ng	139009	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	90
3	Heneicosane	296	C21H44	000629-94-7	83
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	80





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Sample : H5396-07
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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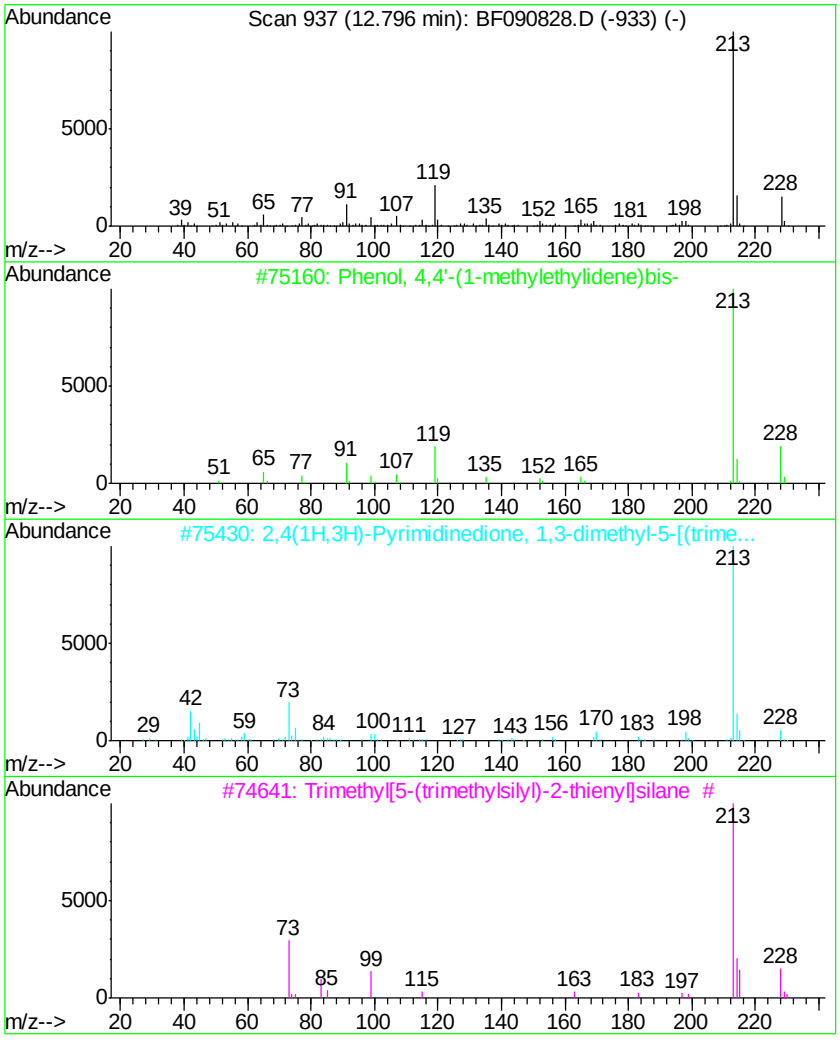
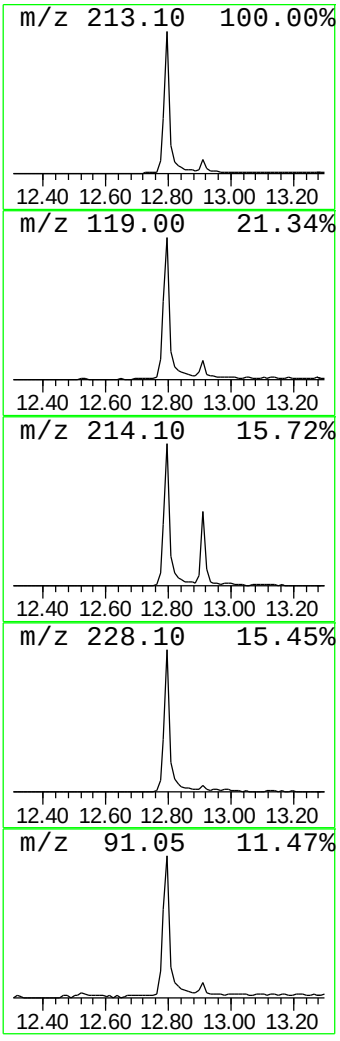
****

Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	17.81 ng	854536	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	50
3	Trimethyl[5-(trimethylsilyl)-2-t...	228	C10H20SSi2	017906-71-7	42
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	40
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	38





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Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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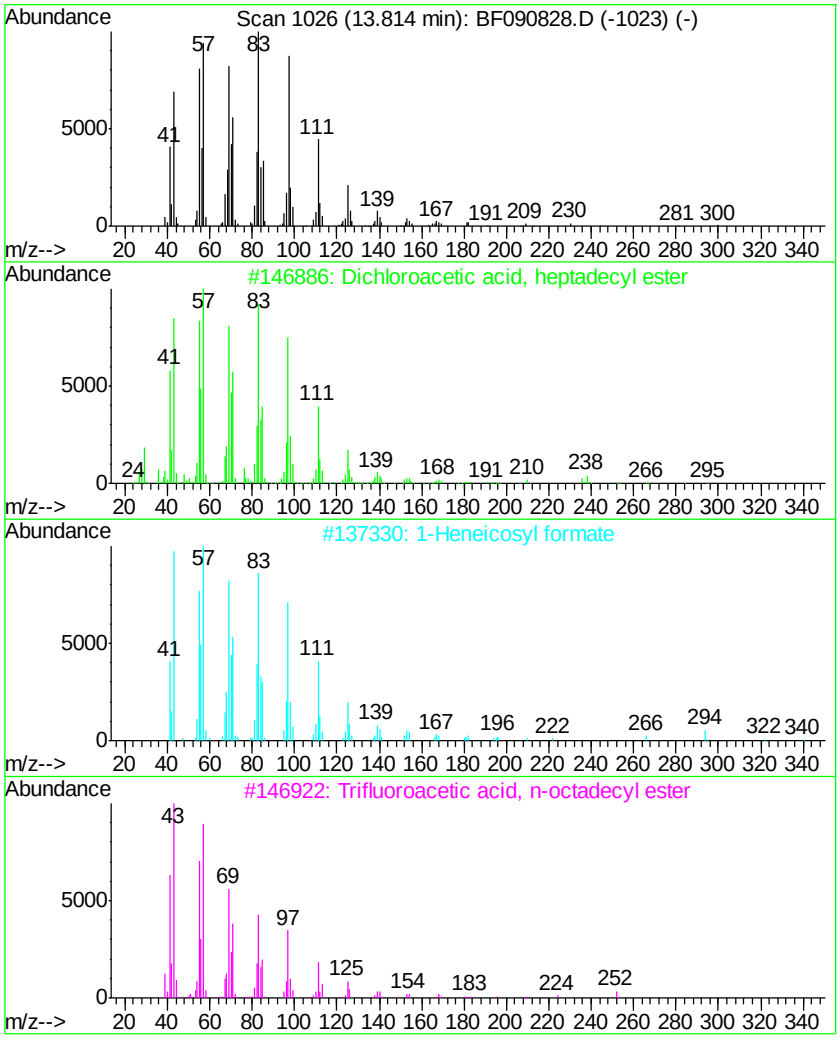
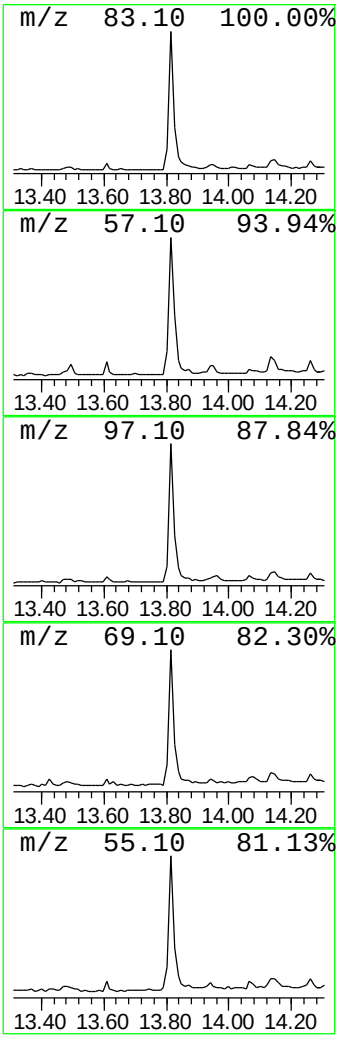
Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	7.19 ng	344840	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91





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Sample : H5396-07
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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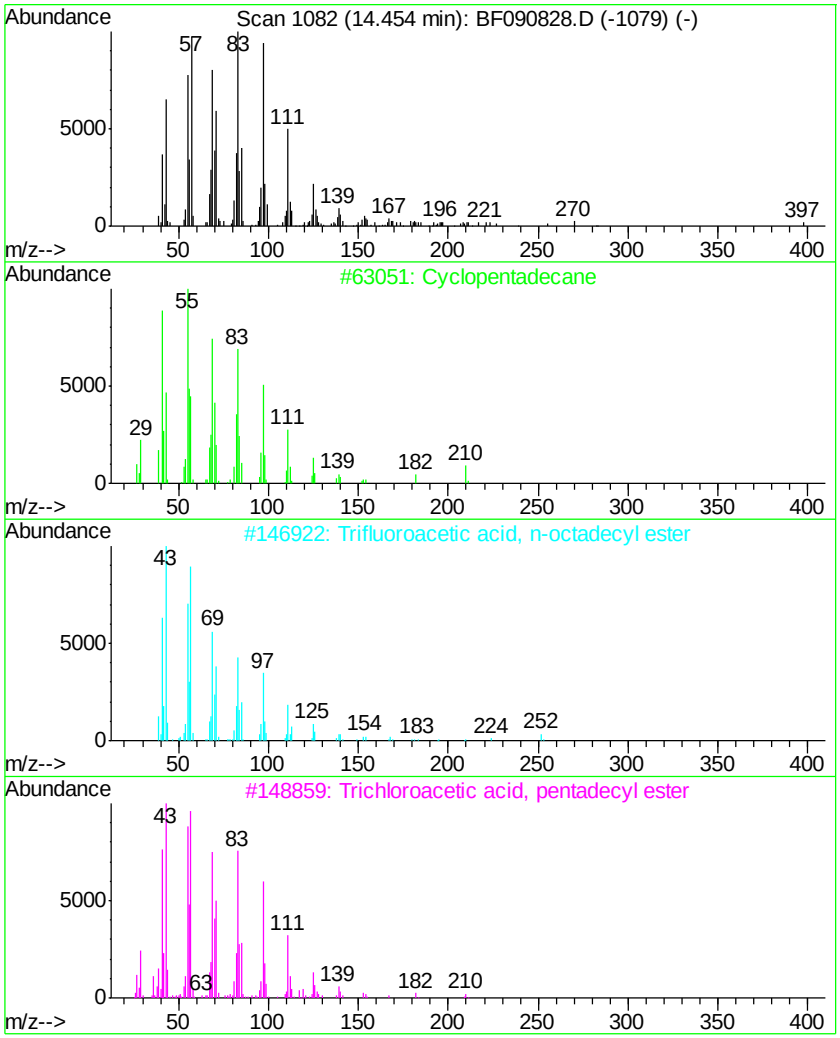
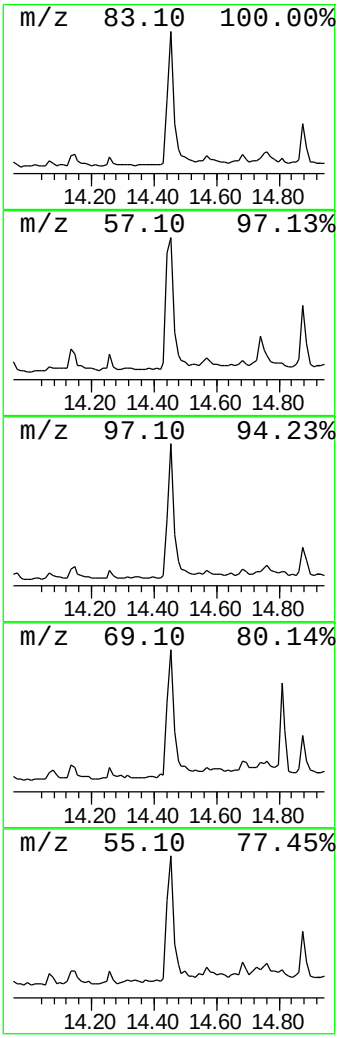
Peak Number 7 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	7.55 ng	362298	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	94
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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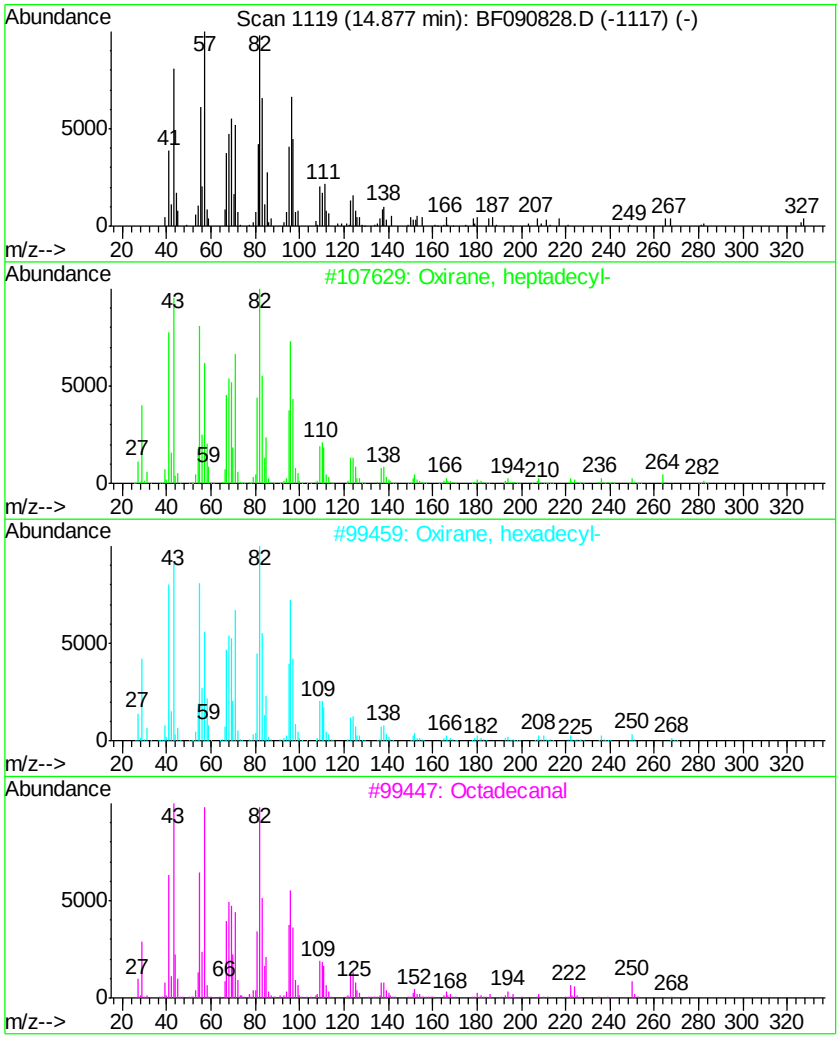
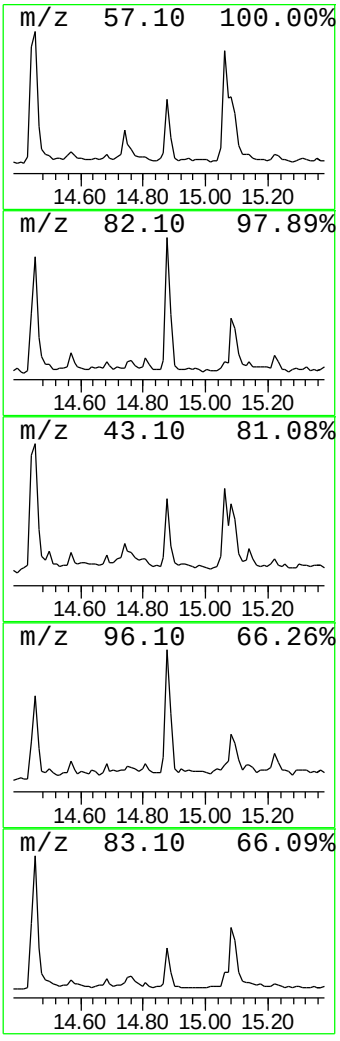
Peak Number 8 Oxirane, heptadecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	2.55 ng	113333	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Tetradecanal	212	C14H28O	000124-25-4	87
5	Pentadecanal-	226	C15H30O	002765-11-9	83





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Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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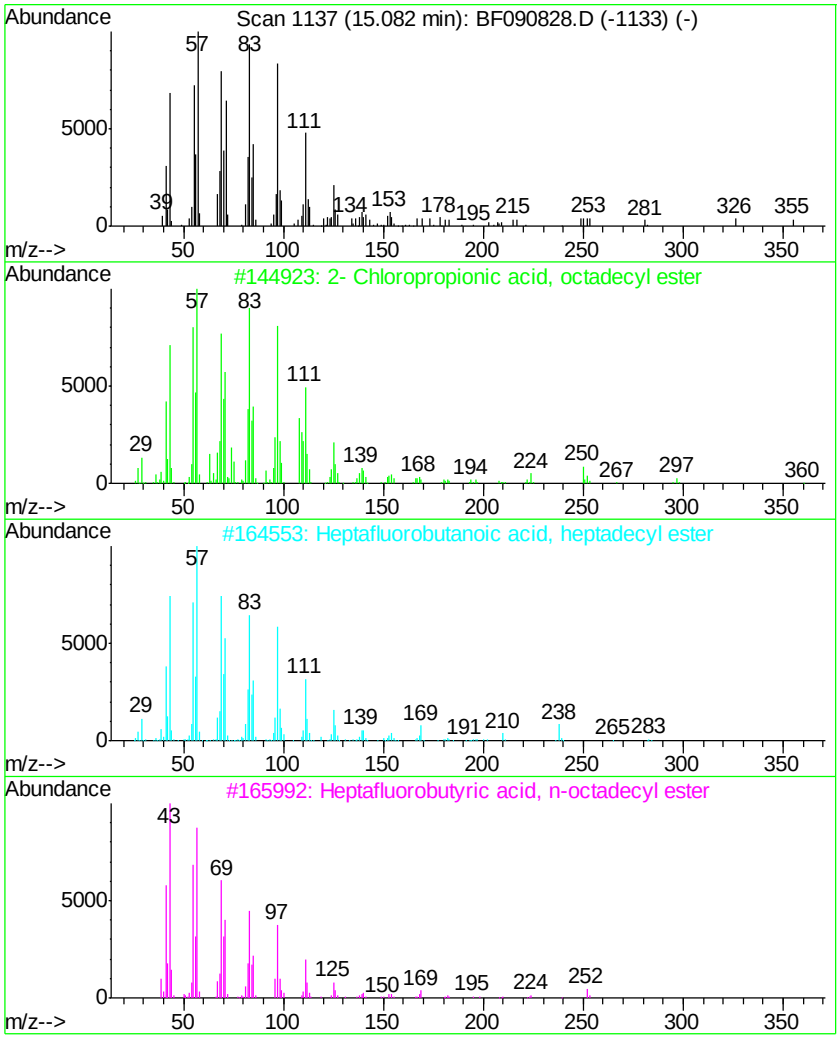
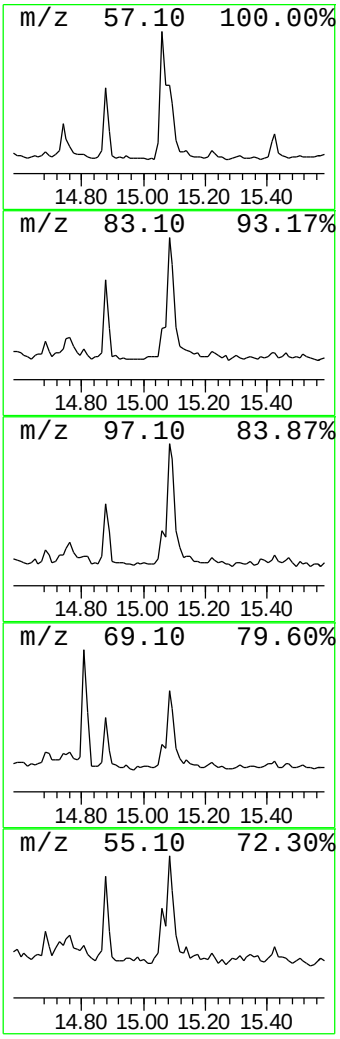
Peak Number 9 2- Chloropropionic acid, oc... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	5.86 ng	260254	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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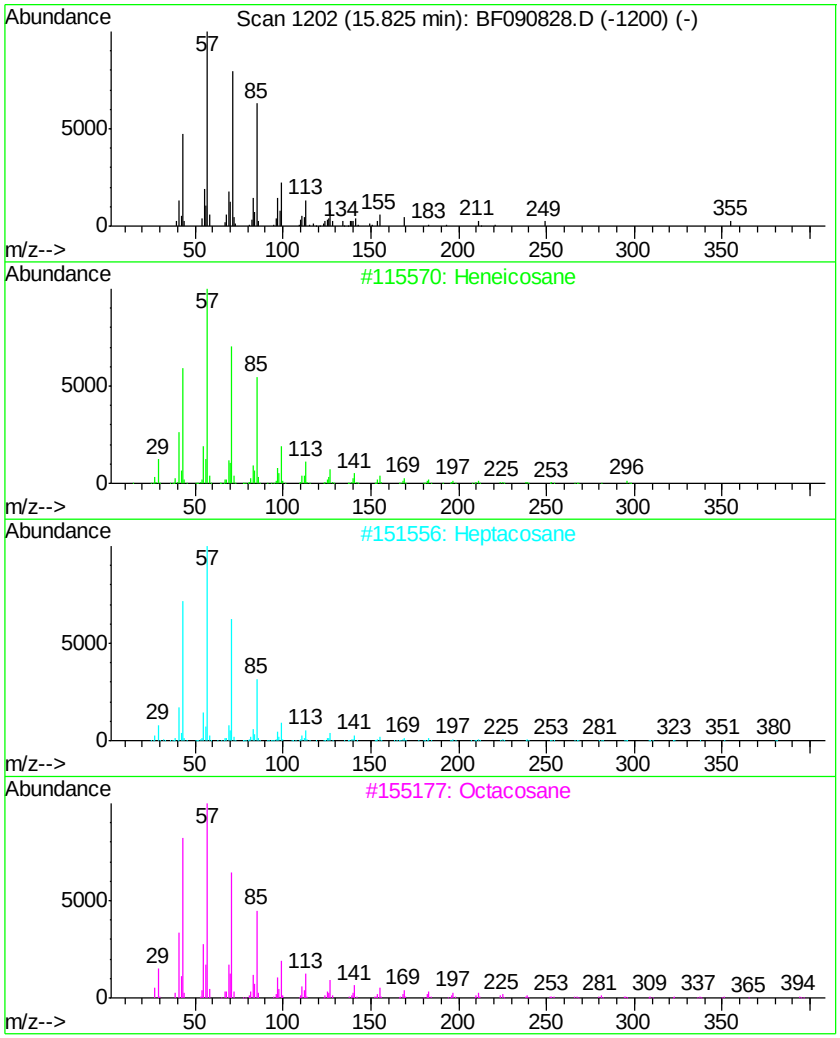
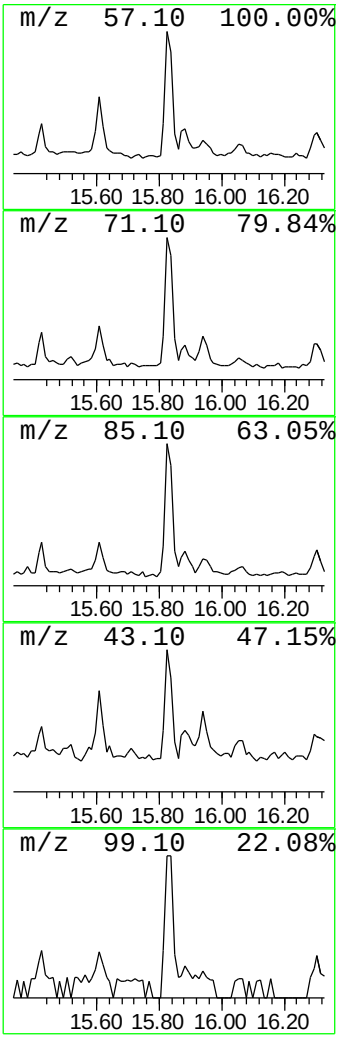
Peak Number 10 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	2.35 ng	104537	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Pentacosane	352	C25H52	000629-99-2	91





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Data File : BF090828.D
Acq On : 26 Oct 2016 00:43
Operator : UM/SJ
Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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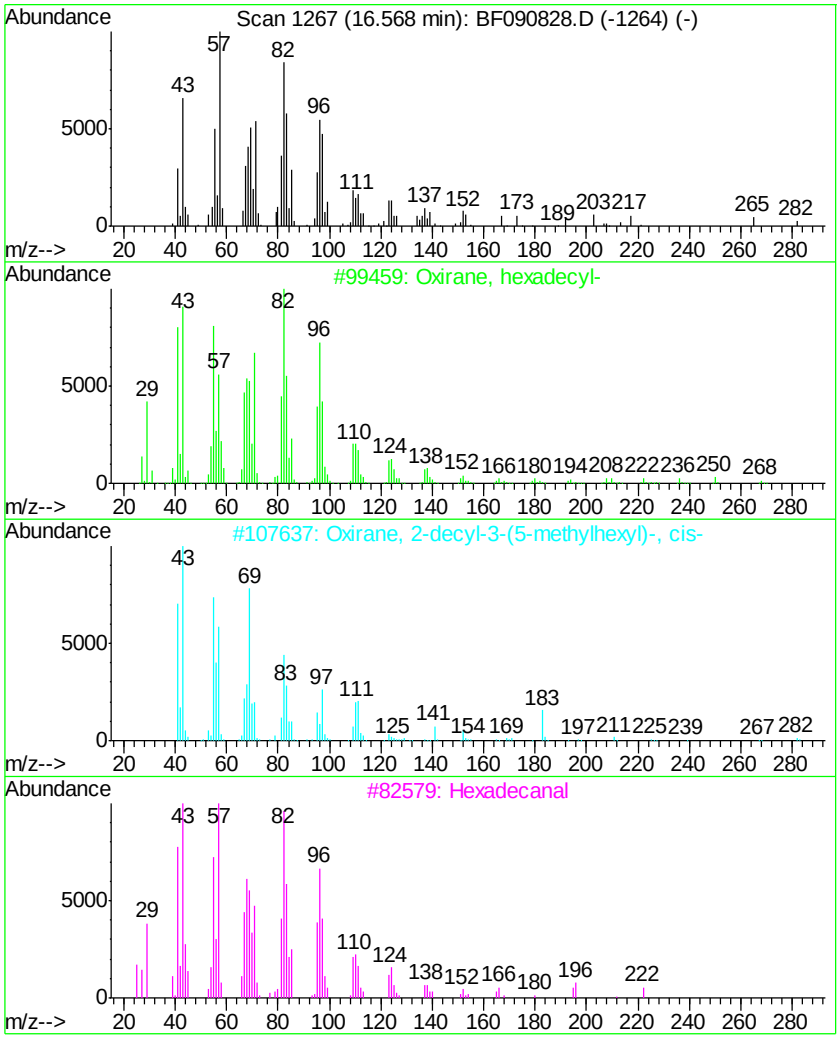
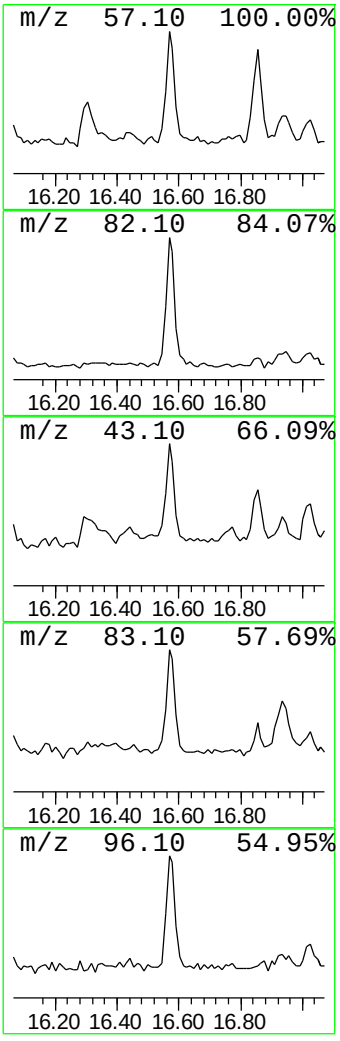
Peak Number 11 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	2.95 ng	131058	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
2	Oxirane, 2-decyl-3-(5-methylhexy...	282	C19H38O	029804-22-6	68
3	Hexadecanal	240	C16H32O	000629-80-1	64
4	16-Octadecenal	266	C18H34O	056554-87-1	64
5	Octadecanal	268	C18H36O	000638-66-4	64





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Operator : UM/SJ
Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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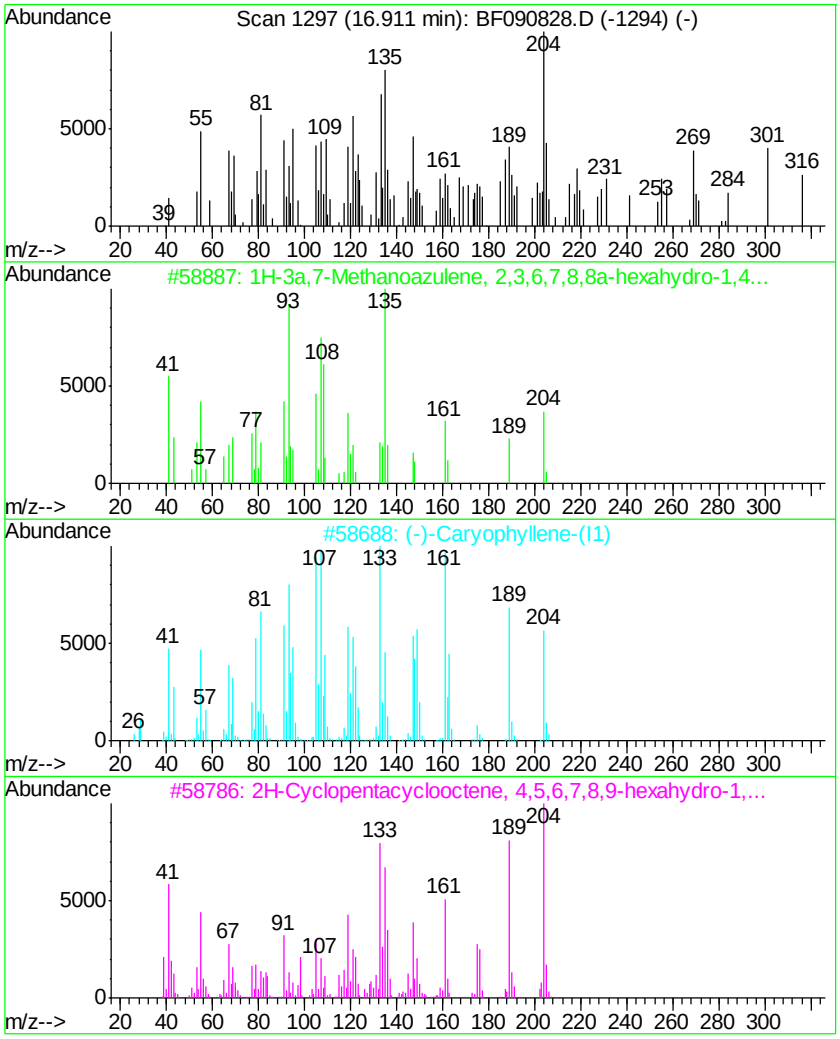
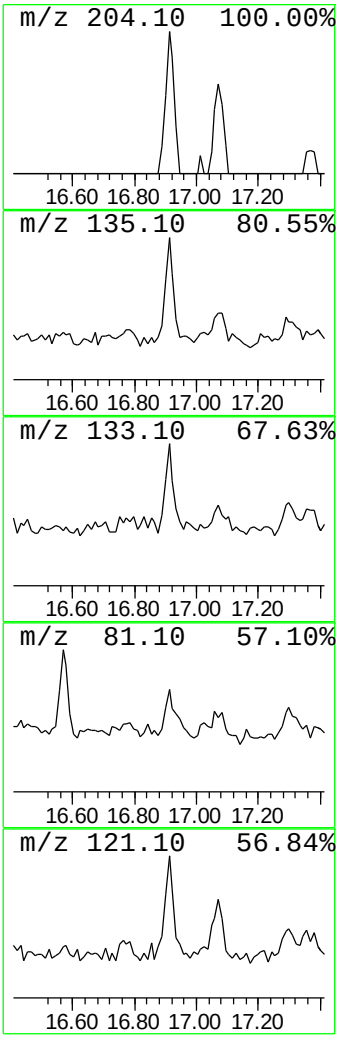
Peak Number 12 unknown16.91 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.91	3.65 ng	162119	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	45
2	(-)-Caryophyllene-(I1)	204	C15H24	1000156-13-1	42
3	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	38
4	.alpha.-D-Glucopyranoside, methy...	482	C19H46O6Si4	002641-79-4	35
5	1,4-Methano-1H-indene, octahydro...	204	C15H24	087064-18-4	27





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Data File : BF090828.D
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Operator : UM/SJ
Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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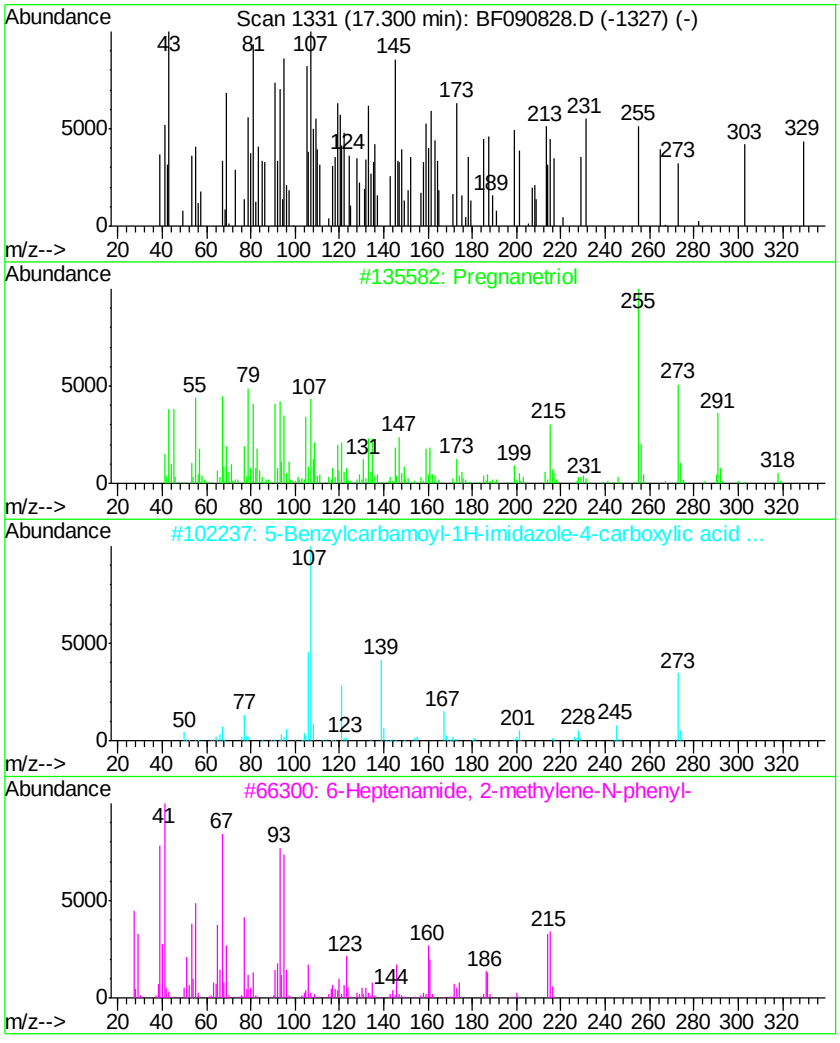
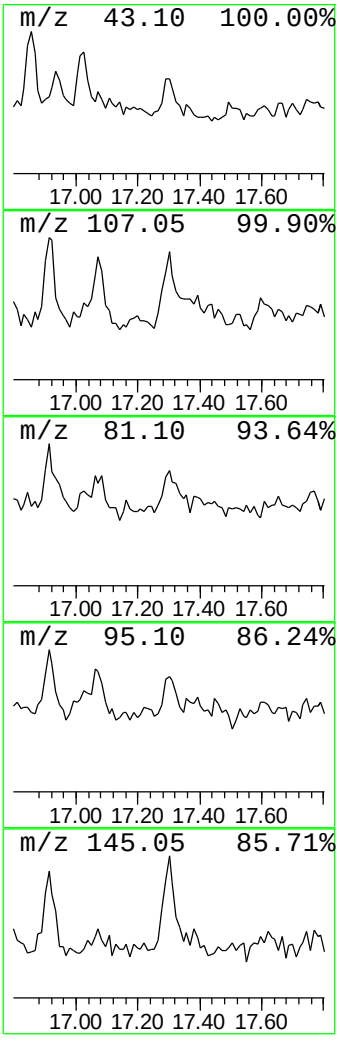
Peak Number 13 unknown17.30 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.17 ng	96342	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pregnanetriol	336	C21H36O3	027178-64-9	10
2	5-Benzylcarbamoyl-1H-imidazole-4...	273	C14H15N3O3	312758-83-1	10
3	6-Heptenamide, 2-methylene-N-phe...	215	C14H17NO	114662-88-3	10
4	Norflurazon	303	C12H9ClF3N3O	027314-13-2	9
5	5-O-Tolylcarbamoyl-3H-imidazole-...	273	C14H15N3O3	313251-31-9	9





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Acq On : 26 Oct 2016 00:43
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Sample : H5396-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P4-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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TIC Library : C:\DATABASE\NIST02.L
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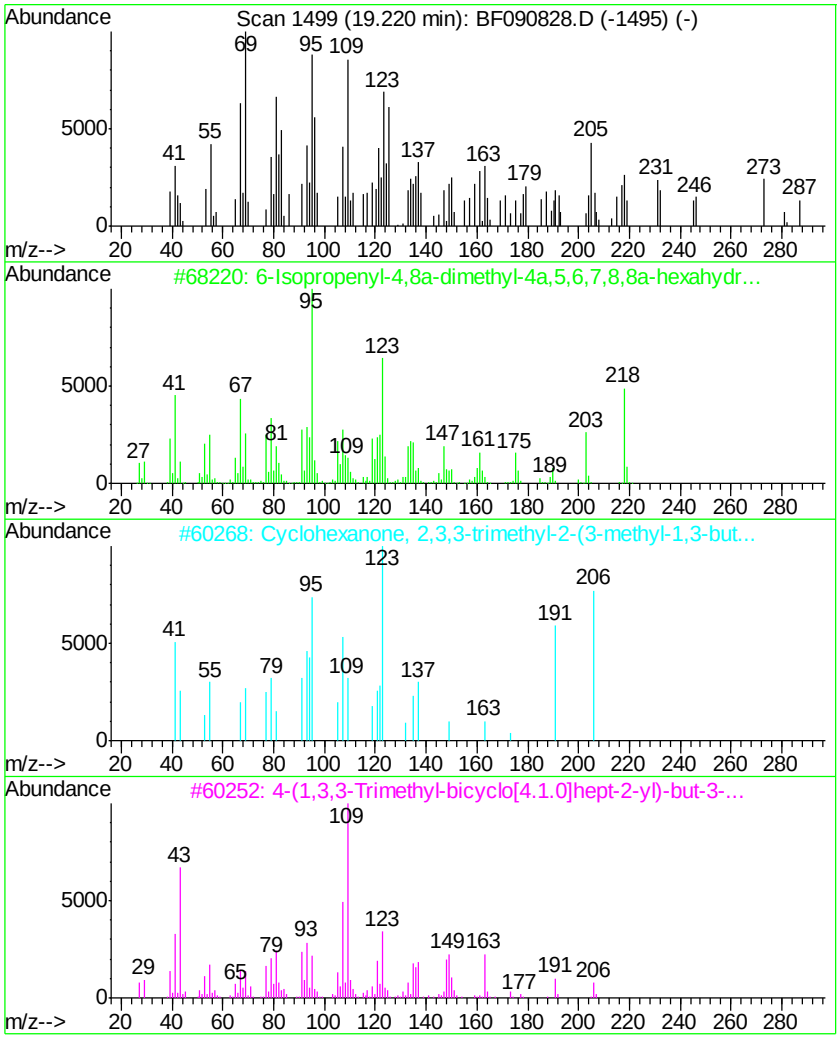
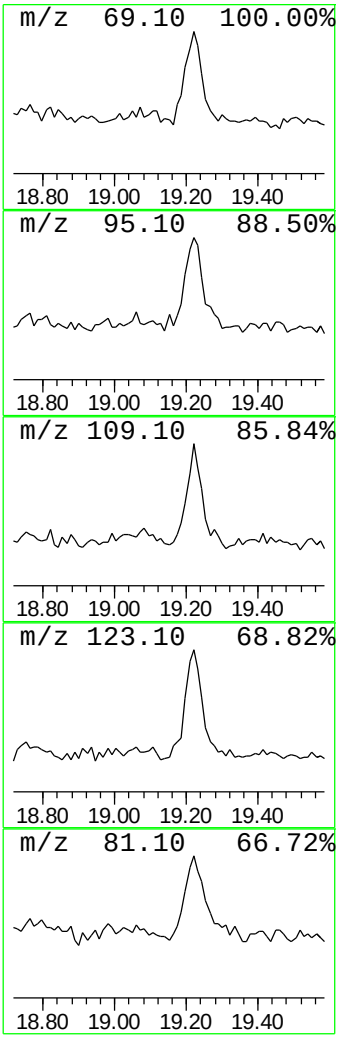
Peak Number 14 6-Isopropenyl-4,8a-dimethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.22	4.41 ng	195961	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	50
2	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	38
3	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	38
4	(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	35
5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	35





Tentatively Identified Compound (LSC) summary

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Data File : BF090828.D
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Operator : UM/SJ
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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
2-Pentanone, 4-hy...	4.97	11.4	ng	613050	1	6.80	1071700	20.0
unknown6.57	6.57	66.2	ng	3544520	1	6.80	1071700	20.0
Hexadecane	10.75	2.1	ng	139009	4	11.32	1314520	20.0
Phenol, 4,4'-(1-m...	12.80	17.8	ng	854536	5	13.96	959720	20.0
Dichloroacetic ac...	13.81	7.2	ng	344840	5	13.96	959720	20.0
Cyclopentadecane	14.45	7.5	ng	362298	5	13.96	959720	20.0
Oxirane, heptadecyl-	14.88	2.5	ng	113333	6	15.38	888293	20.0
2- Chloropropioni...	15.08	5.9	ng	260254	6	15.38	888293	20.0
Heneicosane	15.83	2.4	ng	104537	6	15.38	888293	20.0
Oxirane, hexadecyl-	16.57	3.0	ng	131058	6	15.38	888293	20.0
unknown16.91	16.91	3.6	ng	162119	6	15.38	888293	20.0
unknown17.30	17.30	2.2	ng	96342	6	15.38	888293	20.0
6-Isopropenyl-4,8...	19.22	4.4	ng	195961	6	15.38	888293	20.0