LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
Data File : BF090038.D
Acq On : 8 Sep 2016 21:42
Operator : UM/SJ
Sample : H4704-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-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-BF083116.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	1.724	10	12	65	rVB	4274365	11937797	100.00%	15.762%
2	4.718	272	274	288	rBV	620759	1002704	8.40%	1.324%
3	5.176	311	314	316	rBV	3551173	3773781	31.61%	4.983%
4	6.250	405	408	410	rBV	3473637	4295986	35.99%	5.672%
5	6.364	415	418	420	rBV	3946253	3913037	32.78%	5.166%
6	6.593	436	438	441	rBV	761206	985512	8.26%	1.301%
7	6.753	449	452	455	rBV	3295375	3066344	25.69%	4.049%
8	7.164	485	488	491	rBV	1985633	2273816	19.05%	3.002%
9	7.222	491	493	495	rVV	691176	647892	5.43%	0.855%
10	7.885	548	551	553	rBV	1545260	1420588	11.90%	1.876%
11	8.970	643	646	648	rBV	3747193	4668197	39.10%	6.163%
12	9.359	678	680	683	rBV	1037819	1075498	9.01%	1.420%
13	9.565	696	698	701	rBV2	313863	377518	3.16%	0.498%
14	9.633	701	704	705	rVV	1512754	1534950	12.86%	2.027%
15	9.656	705	706	709	rVB	254209	262707	2.20%	0.347%
16	10.170	749	751	754	rVB	139073	130056	1.09%	0.172%
17	10.410	769	772	775	rBV	2224658	2451648	20.54%	3.237%
18	10.548	782	784	789	rVB2	109678	198068	1.66%	0.262%
19	10.993	822	823	825	rBV	103459	122179	1.02%	0.161%
20	11.119	830	834	837	rBV2	1270839	2811125	23.55%	3.712%
21	11.176	837	839	841	rVV	375256	435395	3.65%	0.575%
22	11.336	849	853	857	rBV2	117369	221914	1.86%	0.293%
23	11.622	873	878	880	rBV2	146211	328641	2.75%	0.434%
24	11.656	880	881	884	rVV2	63253	122799	1.03%	0.162%
25	11.702	884	885	889	rVB	247566	368587	3.09%	0.487%
26	11.896	900	902	907	rVB2	105237	200220	1.68%	0.264%
27	12.308	935	938	940	rBV	1813960	2459597	20.60%	3.247%
28	12.354	940	942	947	rVB3	60849	125834	1.05%	0.166%
29	12.445	947	950	954	rBV	88247	167348	1.40%	0.221%
30	12.525	954	957	960	rBV	2149011	2543643	21.31%	3.358%
31	12.651	966	968	969	rBV	112031	152717	1.28%	0.202%
32	12.685	969	971	973	rVV	3713522	3764514	31.53%	4.970%
33	12.754	973	977	980	rVV3	113282	289941	2.43%	0.383%
34	12.856	982	986	988	rVV	343558	451576	3.78%	0.596%

LSC Area Percent Report

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Acq On : 8 Sep 2016 21:42
Operator : UM/SJ
Sample : H4704-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-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-BF083116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.925	990	992	993	rVV	261165	307419	2.58%	0.406%
36	12.959	993	995	999	rVV2	186569	400708	3.36%	0.529%
37	13.279	1017	1023	1027	rBV3	90564	286552	2.40%	0.378%
38	13.359	1027	1030	1032	rVV2	85578	171168	1.43%	0.226%
39	13.462	1037	1039	1041	rBV	203710	340748	2.85%	0.450%
40	13.496	1041	1042	1047	rVV3	125561	285358	2.39%	0.377%
41	13.588	1049	1050	1053	rVB	138878	189239	1.59%	0.250%
42	13.714	1057	1061	1067	rBV3	1811152	4266690	35.74%	5.633%
43	13.817	1067	1070	1072	rBV	339283	355344	2.98%	0.469%
44	13.919	1077	1079	1080	rBV2	91408	125533	1.05%	0.166%
45	14.102	1090	1095	1096	rVV	210448	339760	2.85%	0.449%
46	14.194	1100	1103	1104	rVV2	128079	165666	1.39%	0.219%
47	14.239	1104	1107	1109	rVB3	149781	298856	2.50%	0.395%
48	14.399	1119	1121	1126	rBV5	98054	274886	2.30%	0.363%
49	14.491	1126	1129	1132	rVV4	164893	355544	2.98%	0.469%
50	14.571	1133	1136	1139	rVV2	150668	263405	2.21%	0.348%
51	14.628	1139	1141	1145	rVV3	60521	142996	1.20%	0.189%
52	14.697	1145	1147	1152	rVV	986379	2182121	18.28%	2.881%
53	14.788	1153	1155	1160	rVV	239926	407942	3.42%	0.539%
54	14.880	1160	1163	1165	rVV3	83697	229488	1.92%	0.303%
55	14.948	1167	1169	1172	rVV	569914	796169	6.67%	1.051%
56	15.005	1172	1174	1176	rVV	916846	1115091	9.34%	1.472%
57	15.062	1176	1179	1189	rVB2	636946	1434731	12.02%	1.894%
58	15.520	1217	1219	1223	rVB	81190	134185	1.12%	0.177%
59	16.125	1268	1272	1278	rBV3	86368	261057	2.19%	0.345%
60	16.262	1281	1284	1289	rVB2	313244	634425	5.31%	0.838%
61	16.628	1312	1316	1324	rBV	267596	615714	5.16%	0.813%
62	16.765	1324	1328	1330	rVV4	44417	123218	1.03%	0.163%
63	16.823	1330	1333	1340	rVB2	84782	223274	1.87%	0.295%
64	18.457	1470	1476	1484	rVB	62399	250450	2.10%	0.331%
65	18.617	1485	1490	1494	rBV2	46398	179554	1.50%	0.237%

Sum of corrected areas: 75739420

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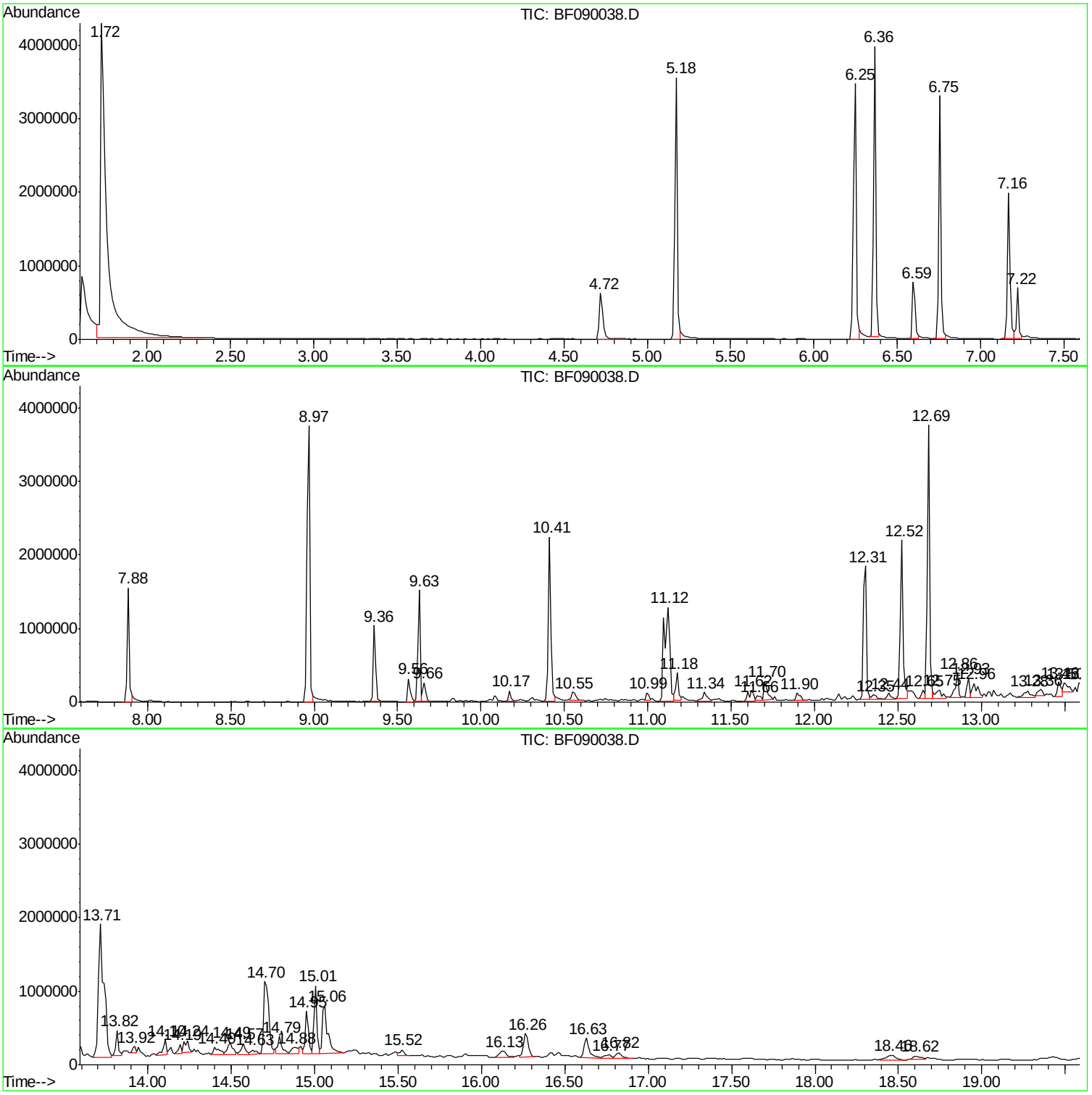
Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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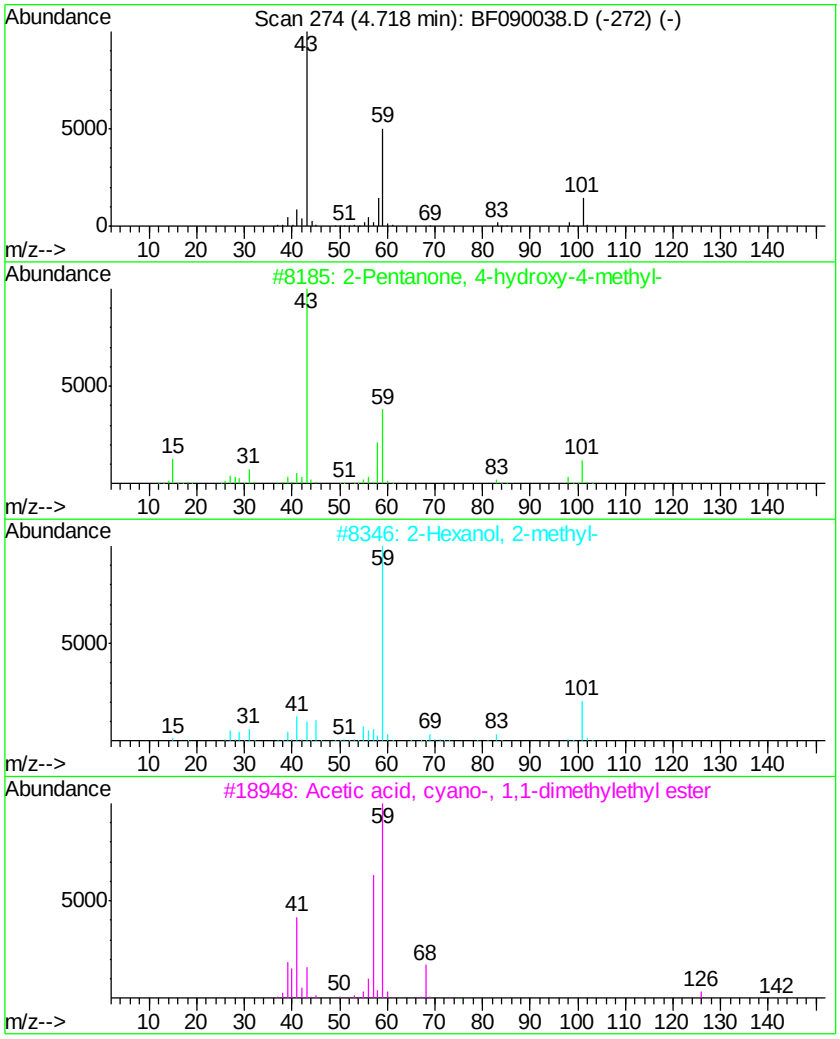
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

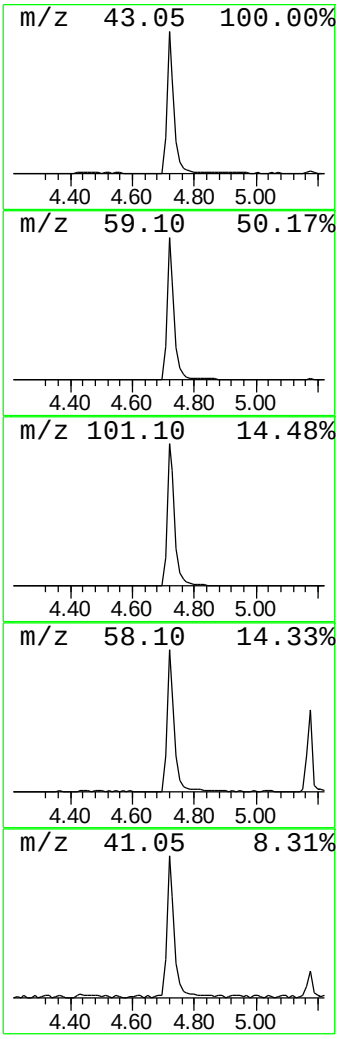
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	20.35 ng	1002700	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Data File : BF090038.D
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Operator : UM/SJ
Sample : H4704-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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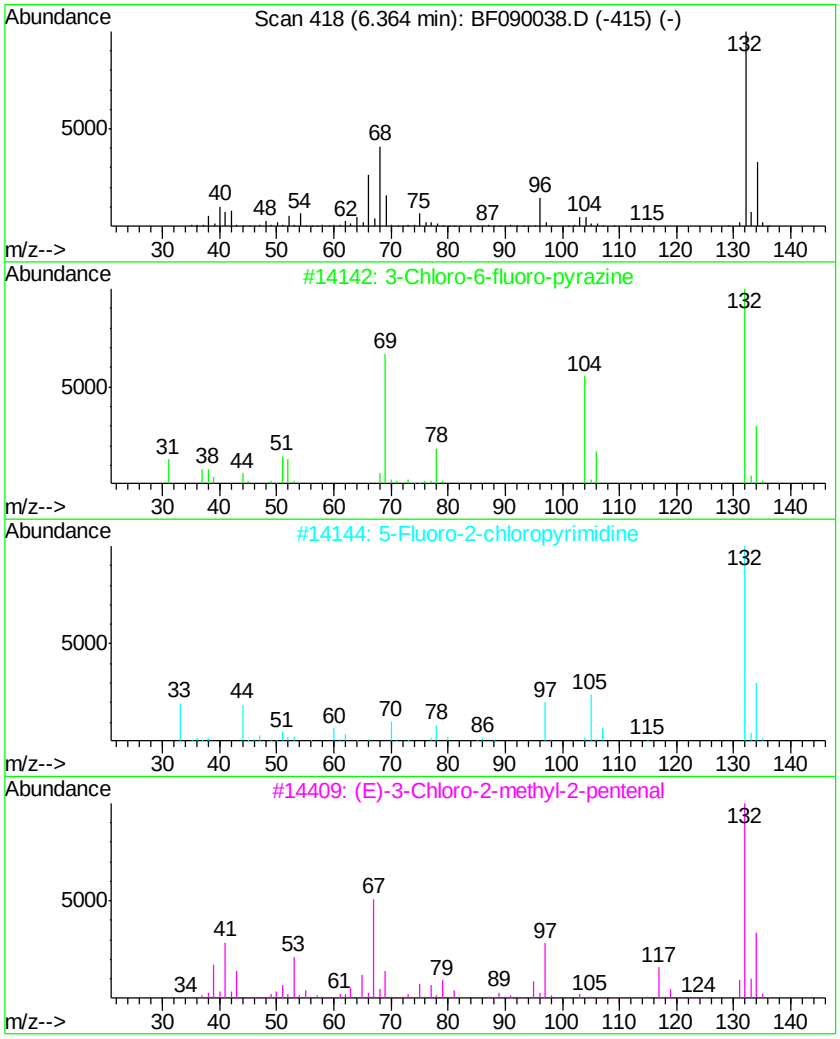
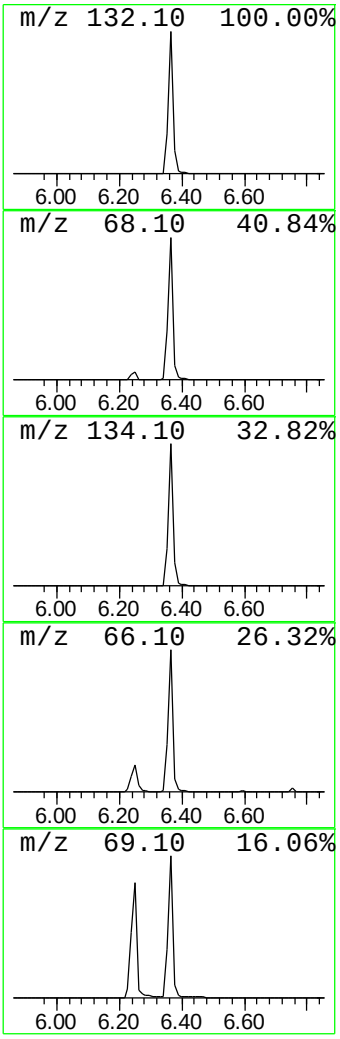
Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	79.41 ng	3913040	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Sample : H4704-09
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
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TIC Library : C:\Database\NIST11.L
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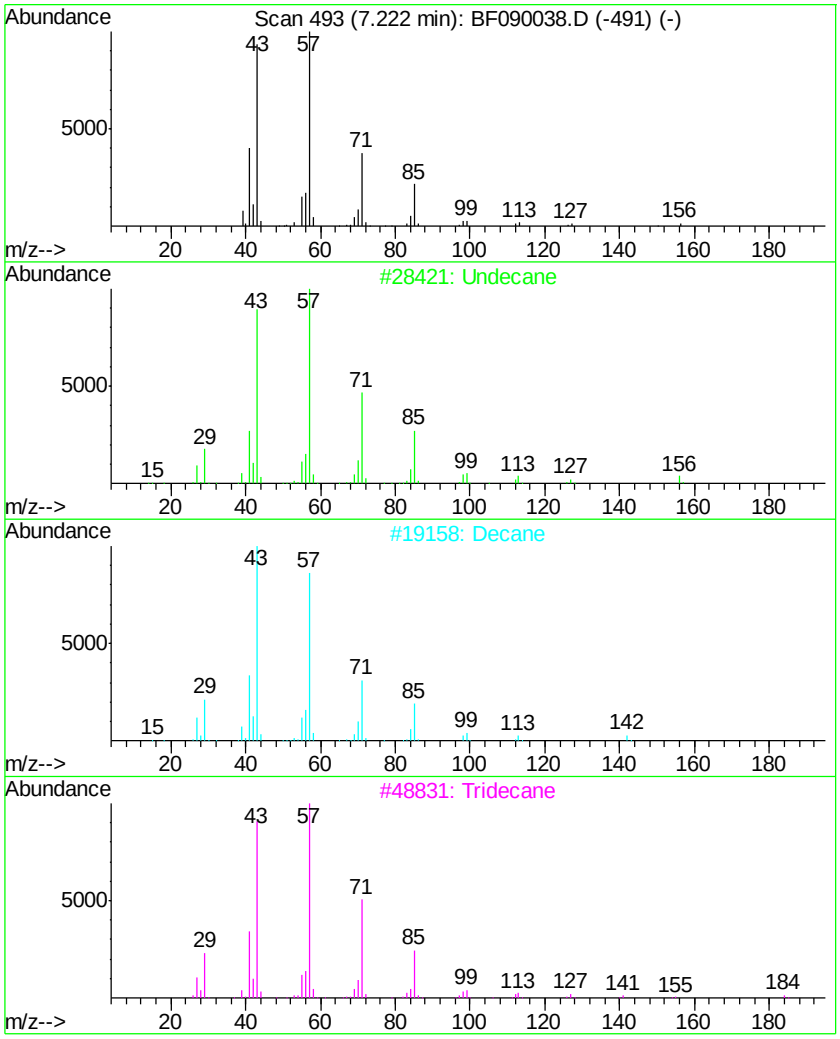
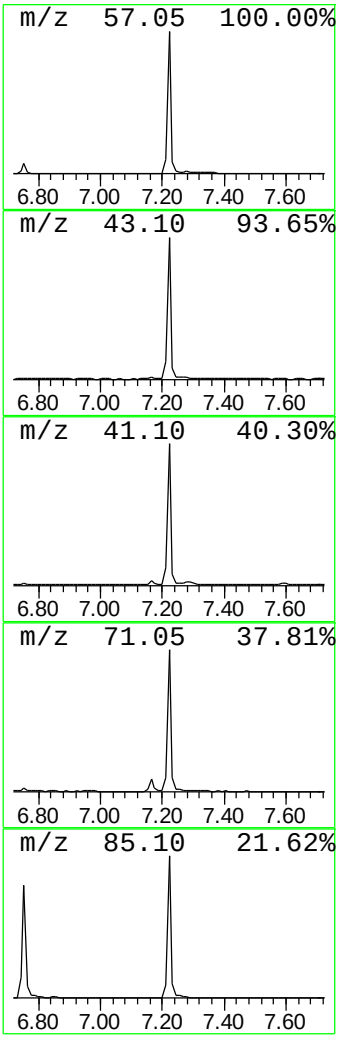
Peak Number 5 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	13.15 ng	647892	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	83
2	Decane	142	C10H22	000124-18-5	78
3	Tridecane	184	C13H28	000629-50-5	78
4	Hexadecane	226	C16H34	000544-76-3	78
5	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	72





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Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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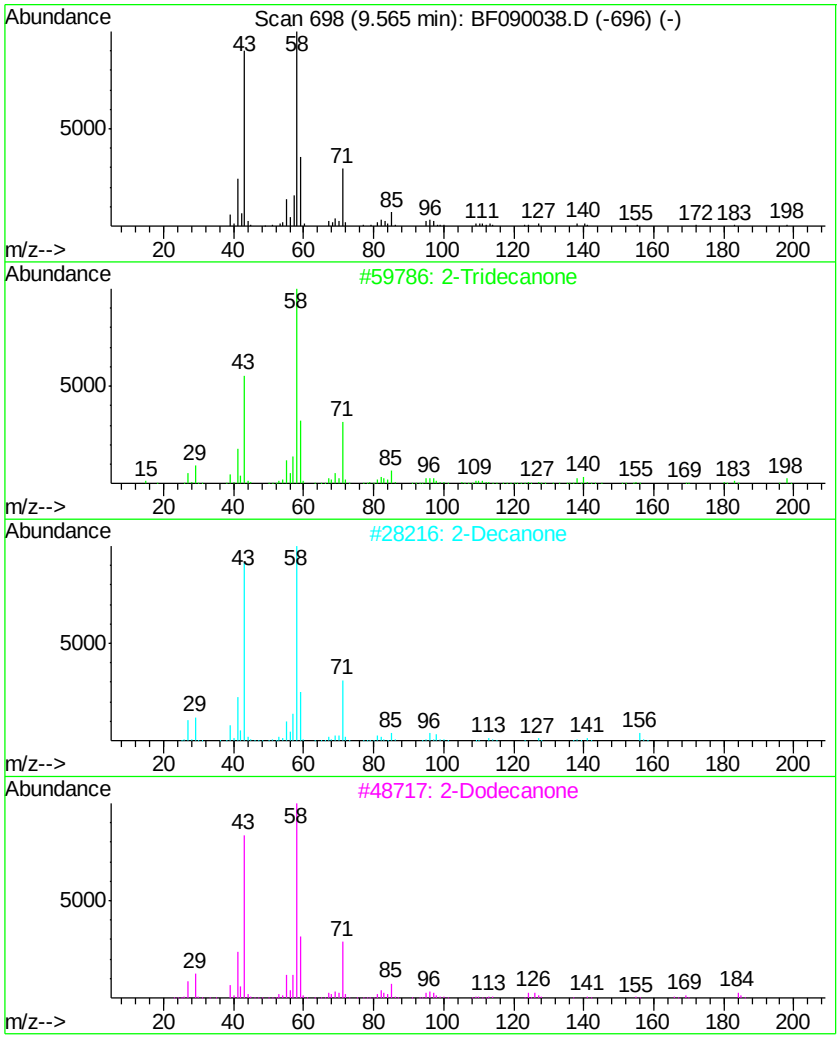
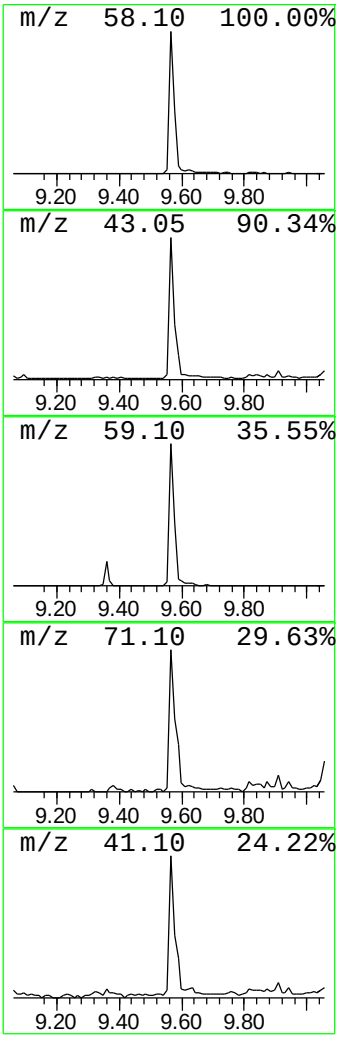
Peak Number 6 2-Tridecanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.56	4.92 ng	377518	Acenaphthene-d10	9.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tridecanone	198	C13H26O	000593-08-8	95
2	2-Decanone	156	C10H20O	000693-54-9	78
3	2-Dodecanone	184	C12H24O	006175-49-1	78
4	2-Tetradecanone	212	C14H28O	002345-27-9	72
5	2-Undecanone	170	C11H22O	000112-12-9	64





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Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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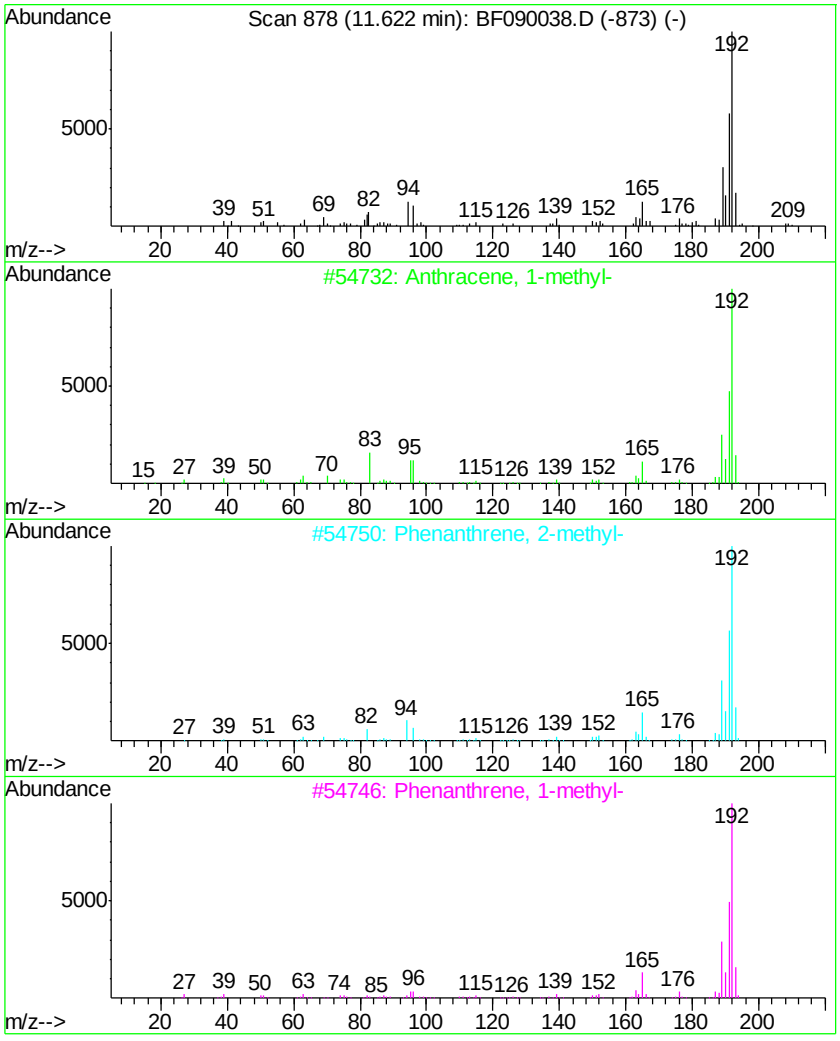
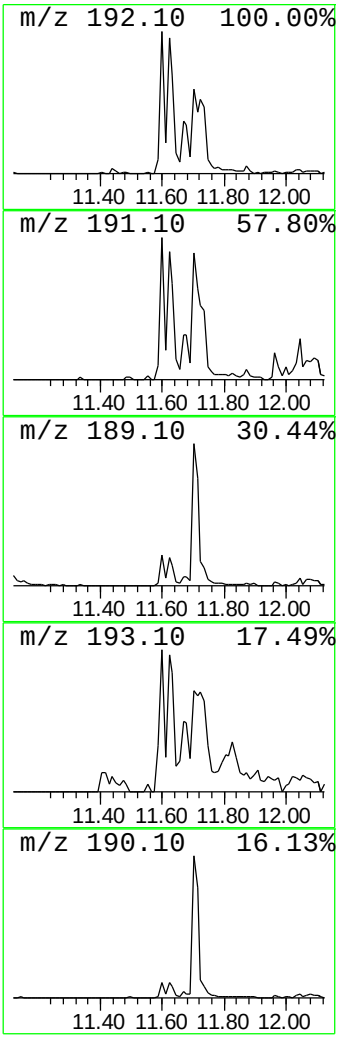
Peak Number 7 Anthracene, 1-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	2.34 ng	328641	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	90





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Sample : H4704-09
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Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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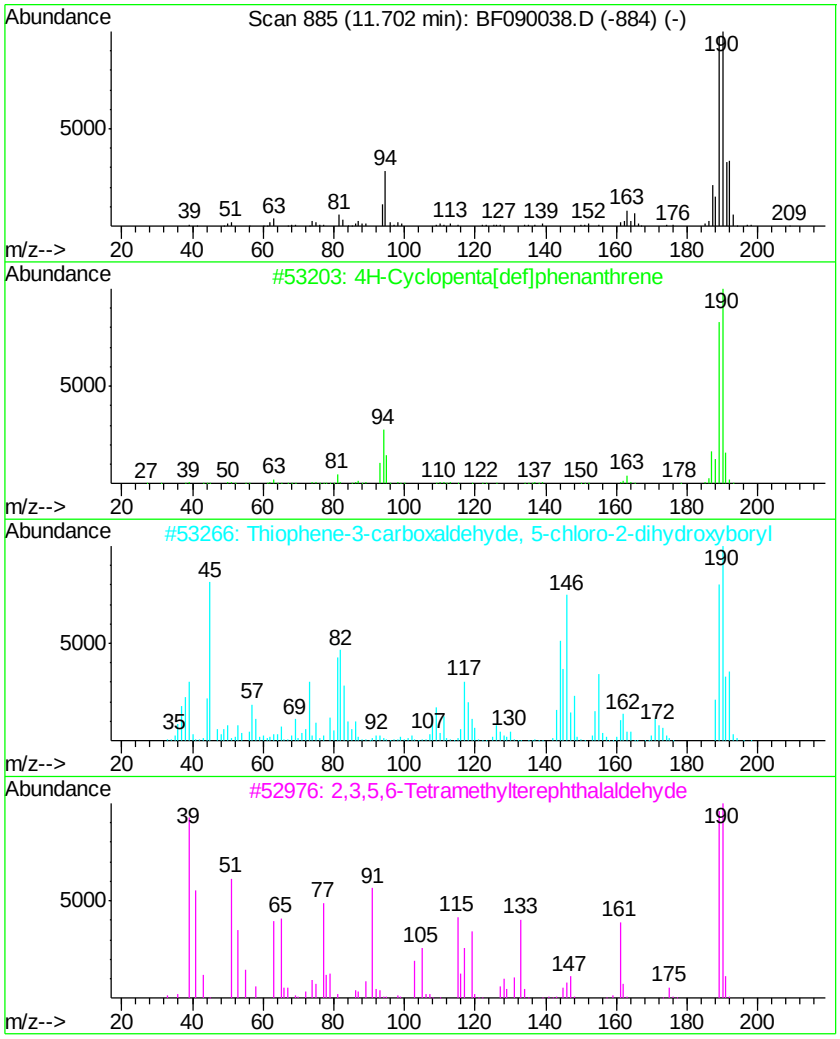
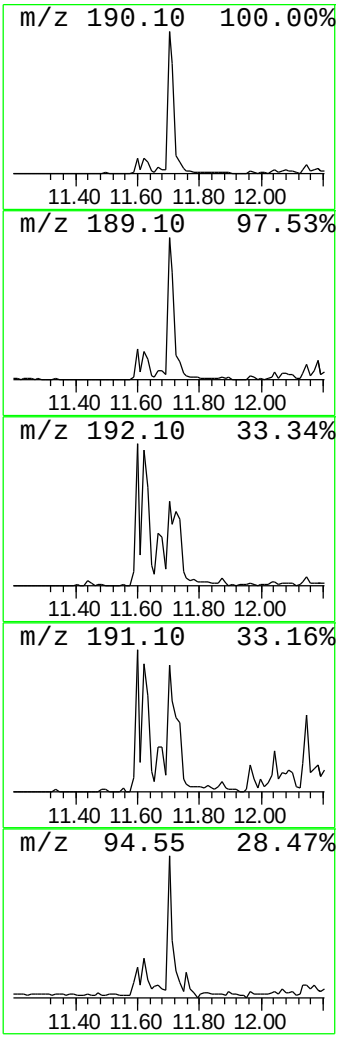
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	2.62 ng	368587	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	49
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
4	Methyl diselenide	190	C2H6Se2	007101-31-7	45
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28





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Operator : UM/SJ
Sample : H4704-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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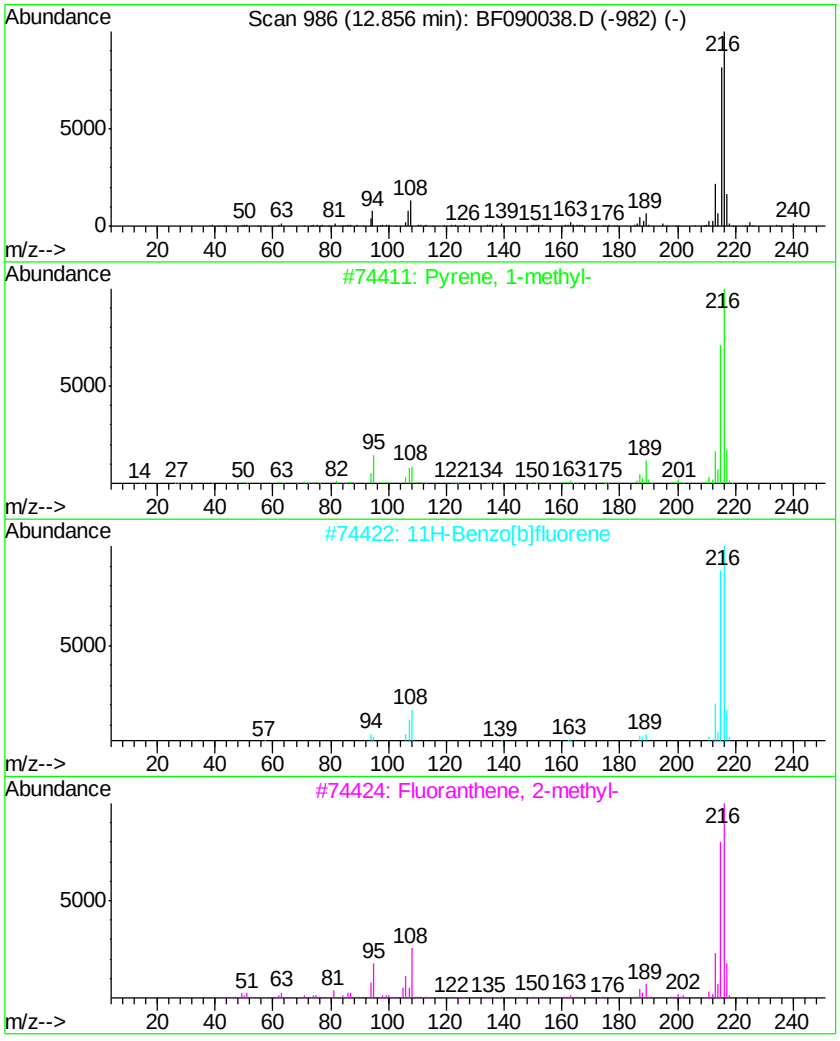
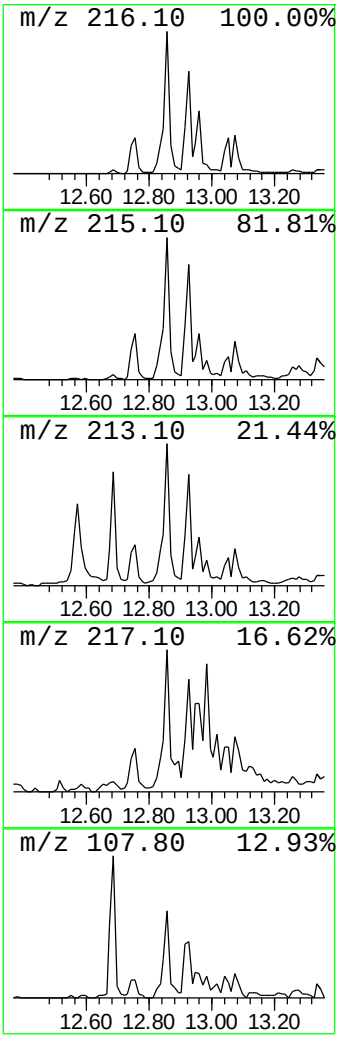
Peak Number 9 Pyrene, 1-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	2.12 ng	451576	Chrysene-d12	13.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





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Misc :
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Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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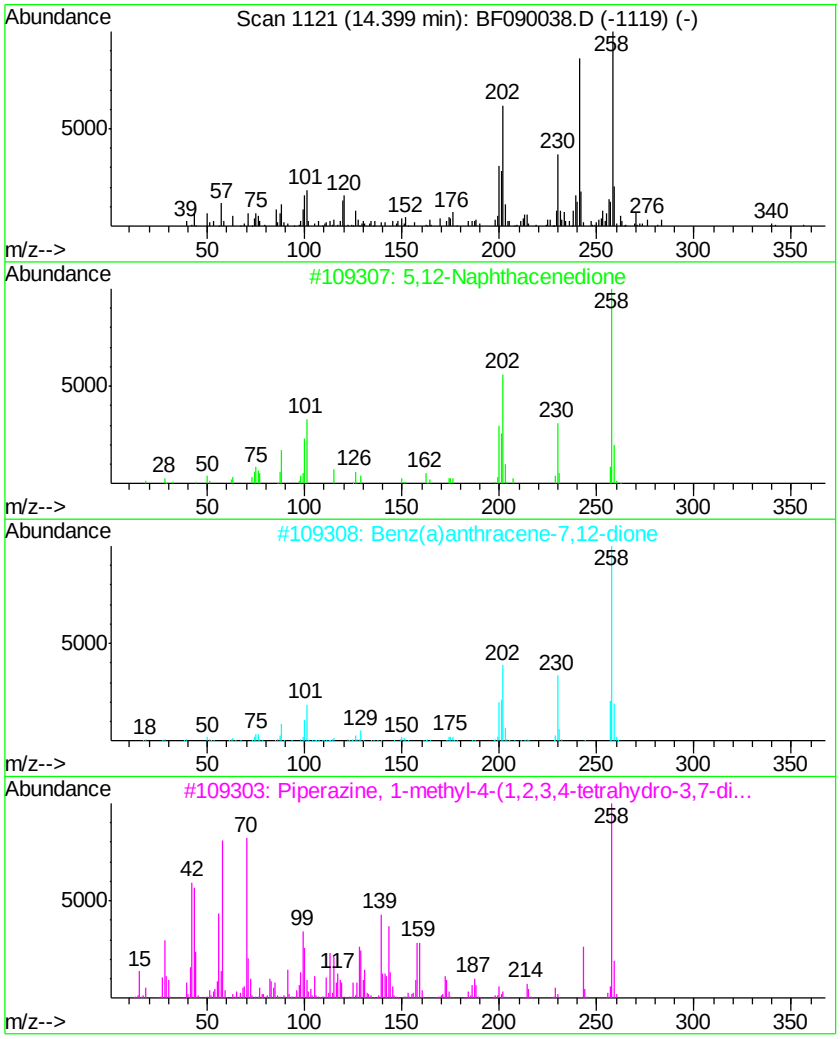
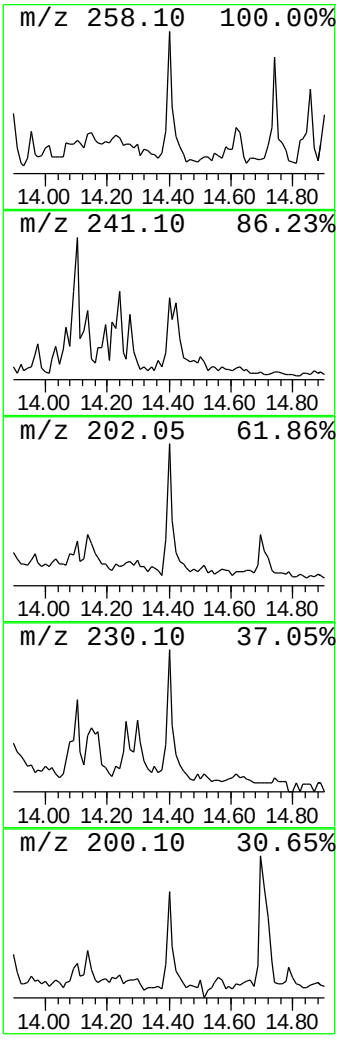
Peak Number 10 5,12-Naphthacenedione Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	3.83 ng	274886	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,12-Naphthacenedione	258	C18H10O2	001090-13-7	98
2	Benz(a)anthracene-7,12-dione	258	C18H10O2	002498-66-0	83
3	Piperazine, 1-methyl-4-(1,2,3,4-...	258	C17H26N2	055591-14-5	56
4	1,8-Anthracenedinitrile, 9,10-di...	258	C16H6N2O2	090866-50-5	46
5	Benzenamine, 4-(9H-carbazol-9-yl)-	258	C18H14N2	052708-37-9	43





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Data File : BF090038.D
Acq On : 8 Sep 2016 21:42
Operator : UM/SJ
Sample : H4704-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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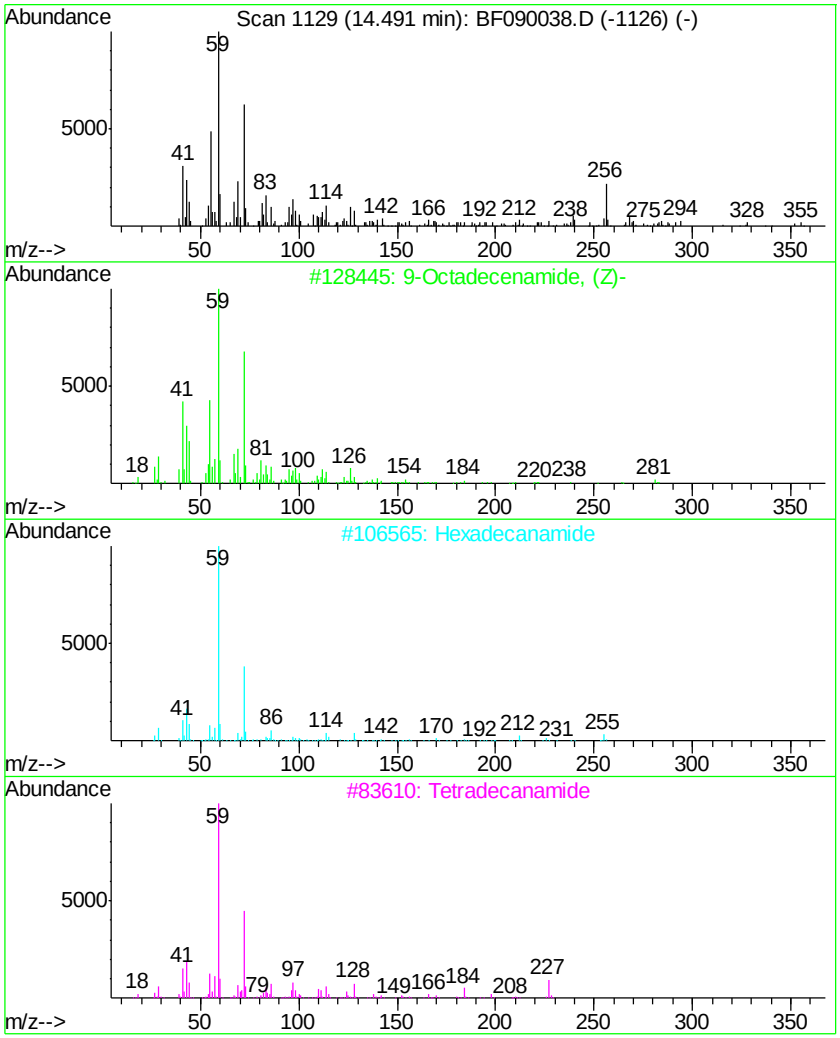
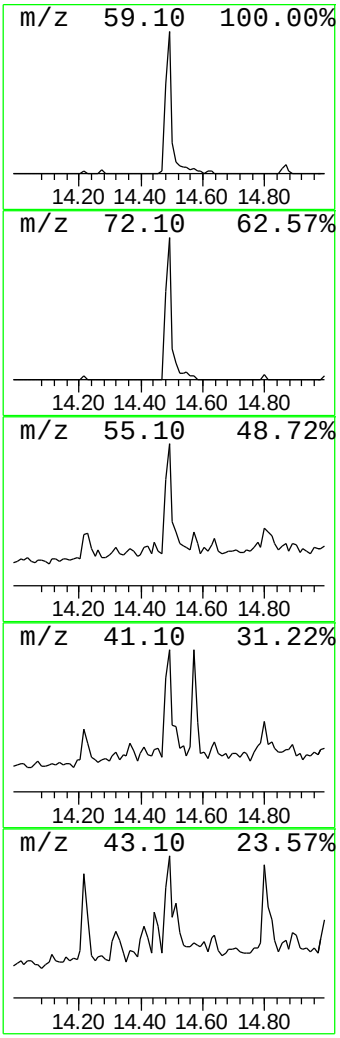
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	4.96 ng	355544	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	Hexadecanamide	255	C16H33NO	000629-54-9	70
3	Tetradecanamide	227	C14H29NO	000638-58-4	59
4	Octadecanamide	283	C18H37NO	000124-26-5	38
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	38





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TIC Library : C:\Database\NIST11.L
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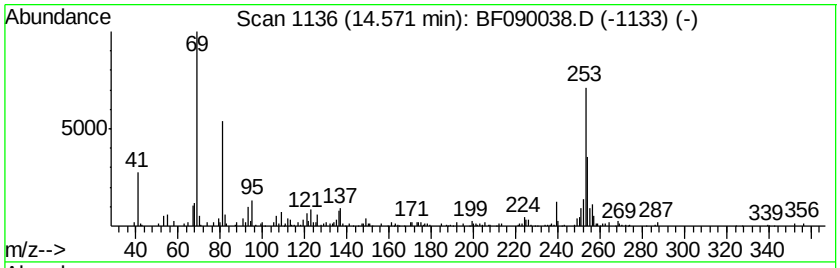
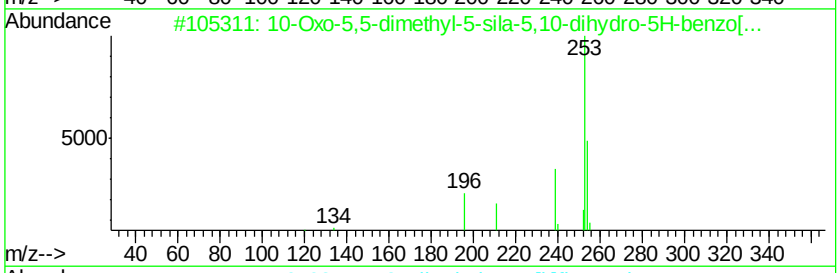
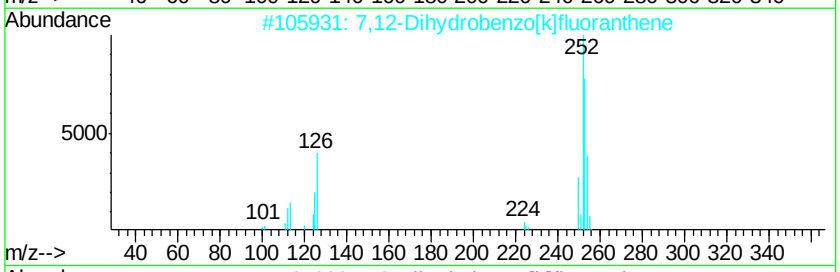
Peak Number 12 10-Oxo-5,5-dimethyl-5-sila-... Concentration Rank 11

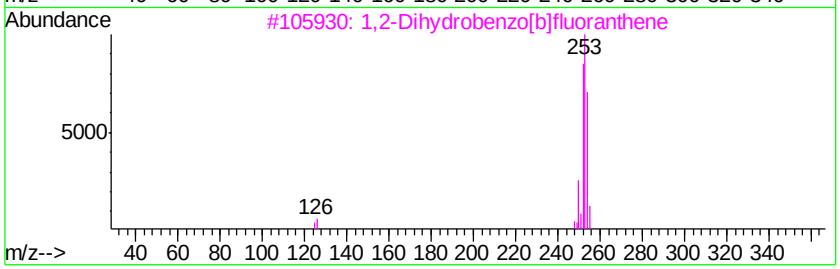
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.67 ng	263405	Perylene-d12	15.06

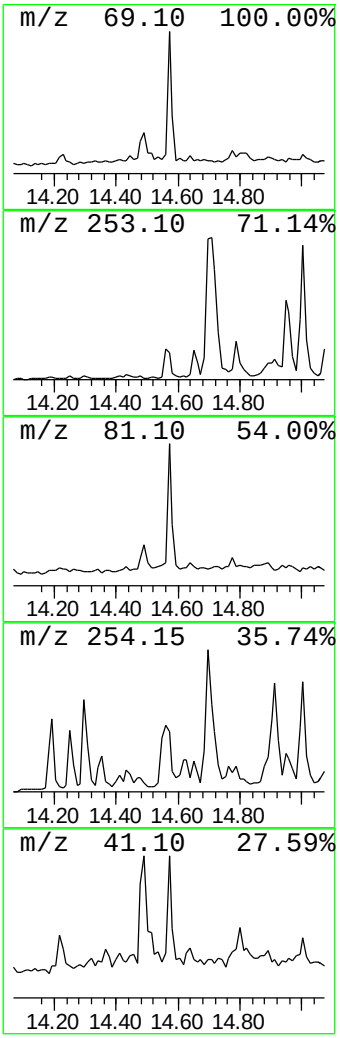
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Oxo-5,5-dimethyl-5-sila-5,10-...	254	C14H14N2OSi	089052-45-9	59
2	7,12-Dihydrobenzo[k]fluoranthene	254	C20H14	1000080-17-7	58
3	1,2-Dihydrobenzo[b]fluoranthene	254	C20H14	100516-13-0	53
4	1,1'-Binaphthalene	254	C20H14	000604-53-5	43
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	42











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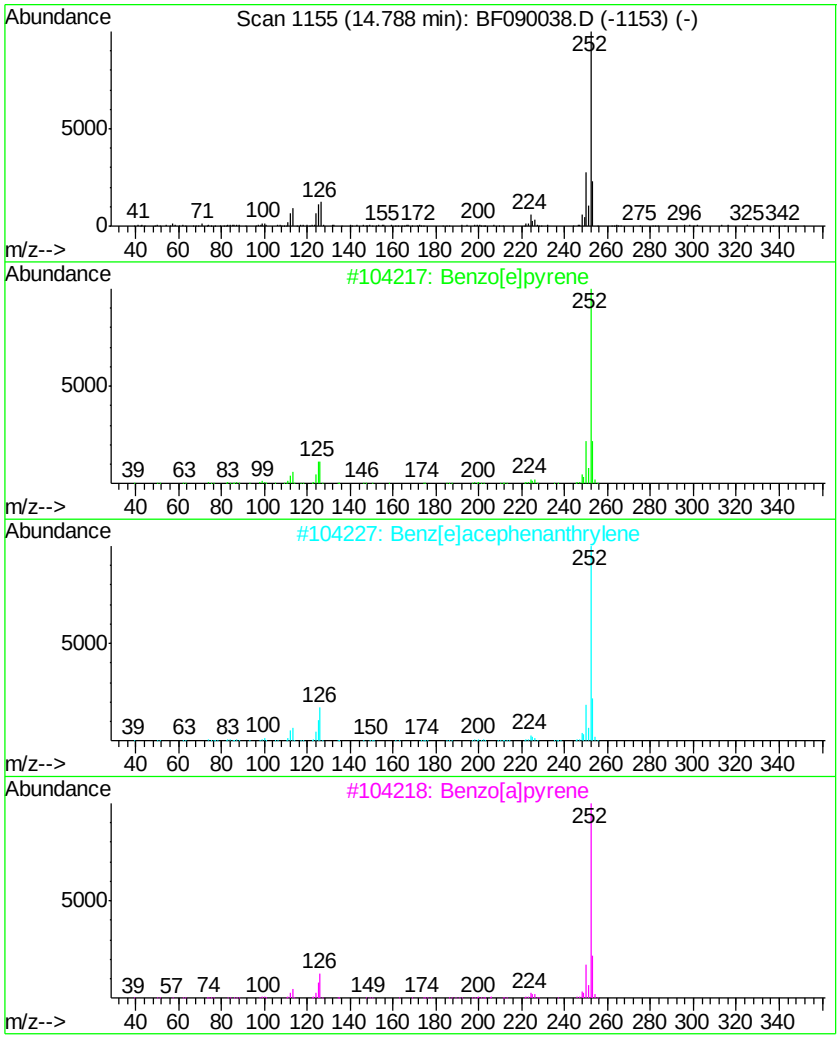
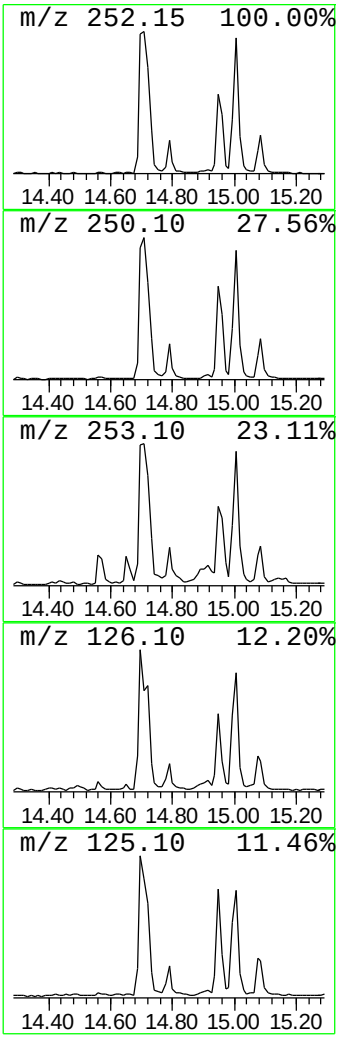
Peak Number 13 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	5.69 ng	407942	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Perylene	252	C20H12	000198-55-0	87





Library Search Compound Report

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BNA_F
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COMP-1

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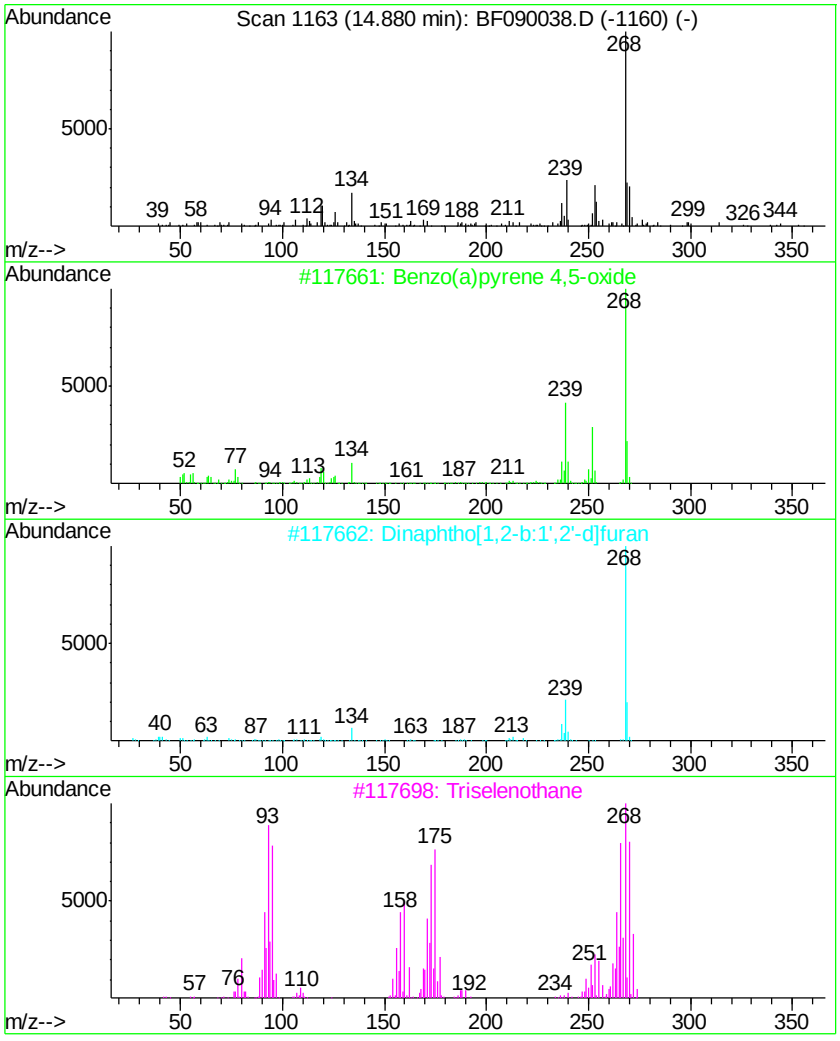
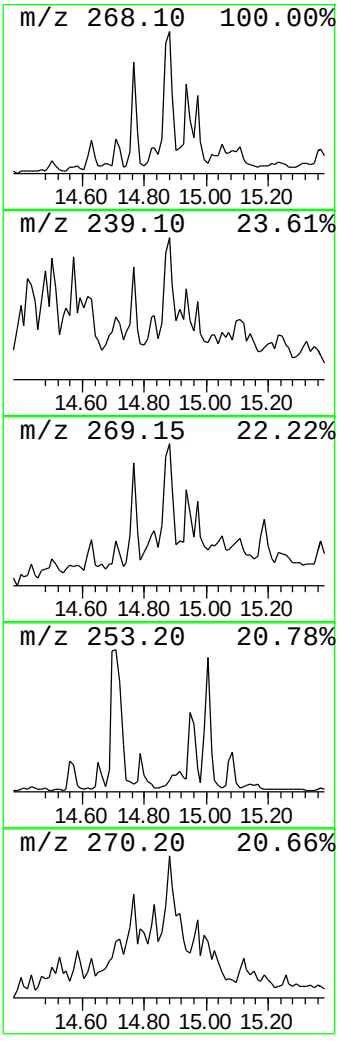
Peak Number 14 Benzo(a)pyrene 4,5-oxide Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	3.20 ng	229488	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo(a)pyrene 4,5-oxide	268	C20H12O	037574-47-3	62
2	Dinaphtho[1,2-b:1',2'-d]furan	268	C20H12O	000207-93-2	58
3	Triselenothane	268	C2H4Se3	121400-83-7	55
4	trans-4'-Methyl-4-(methylthio)ch...	268	C17H16OS	126443-27-4	53
5	Dinaphtho[2,1-b:1',2'-d]furan	268	C20H12O	000194-63-8	52





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Instrument : BNA_F
ClientSampleId : COMP-1

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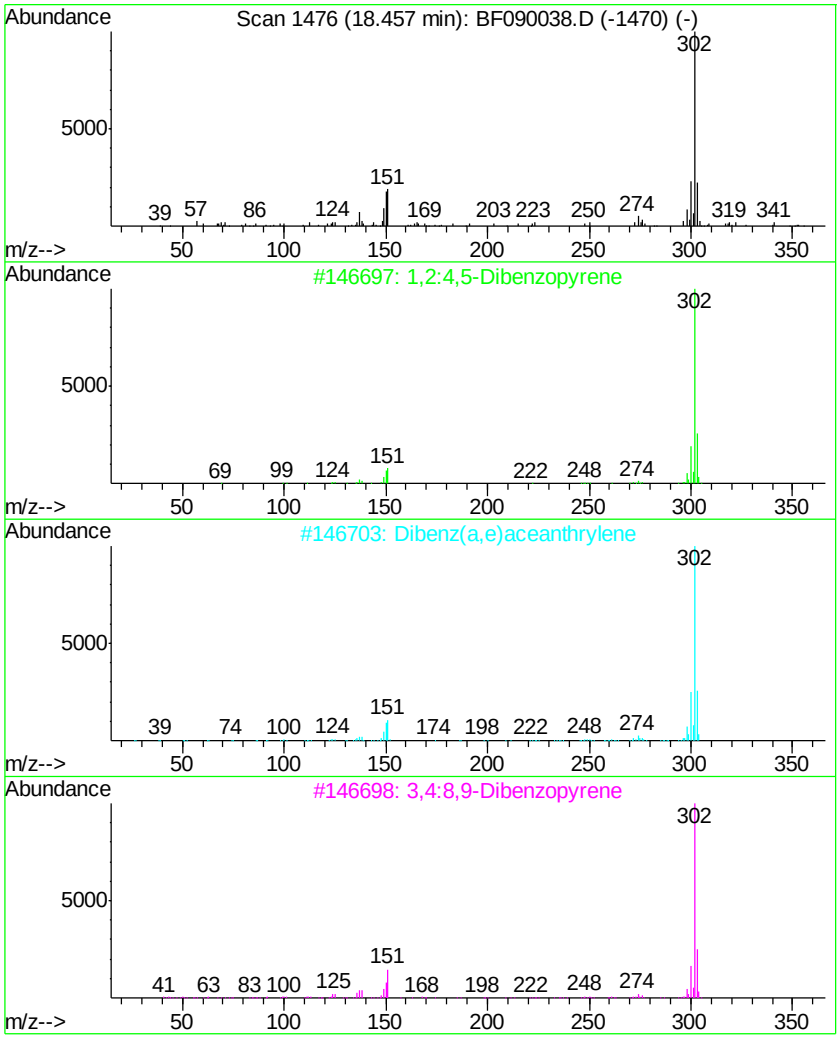
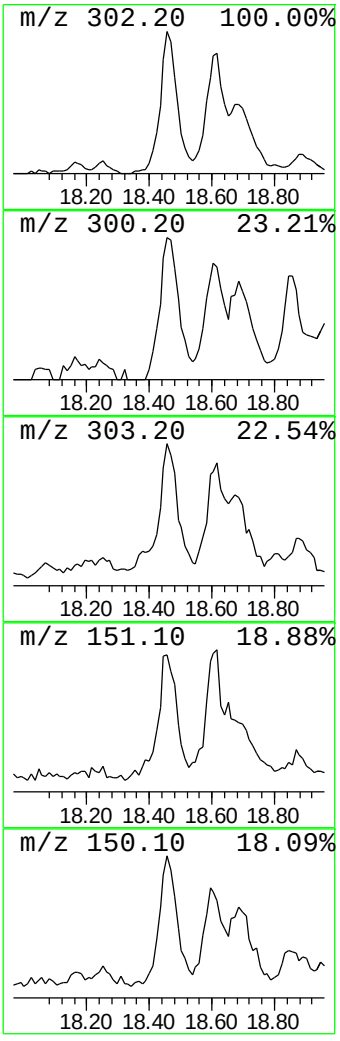
Peak Number 18 1,2:4,5-Dibenzopyrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.46	3.49 ng	250450	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	95
2	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	95
3	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	90
4	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	90
5	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	62





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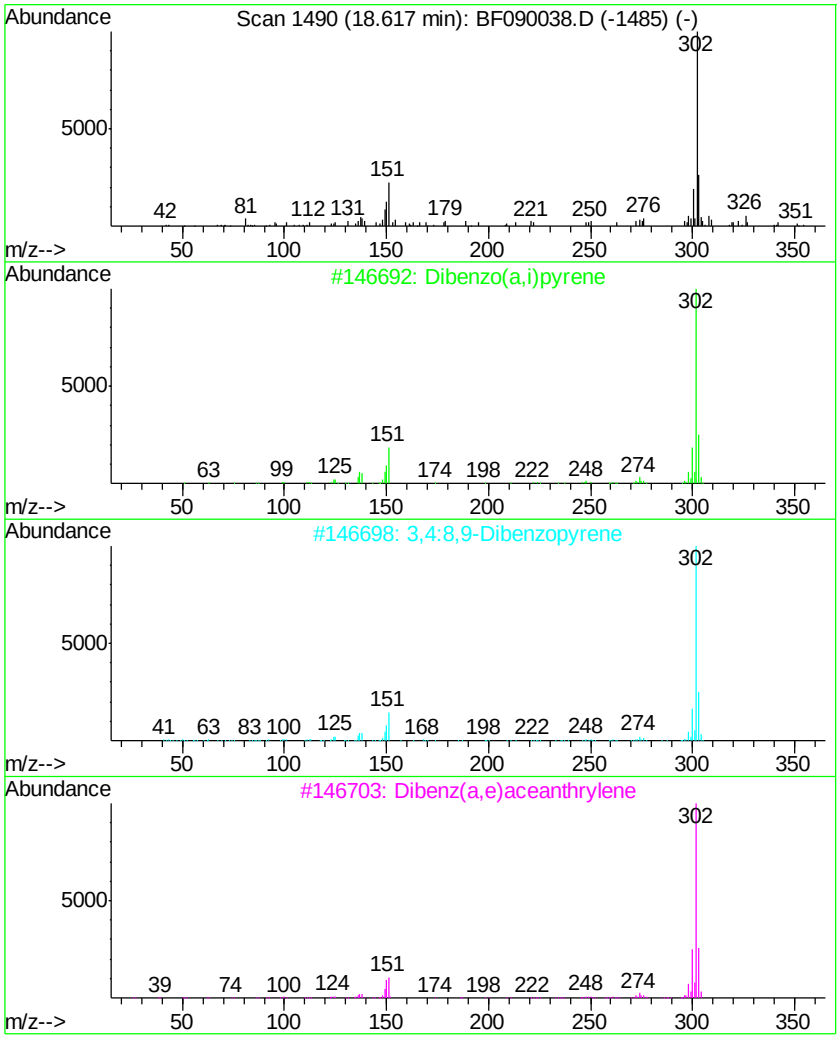
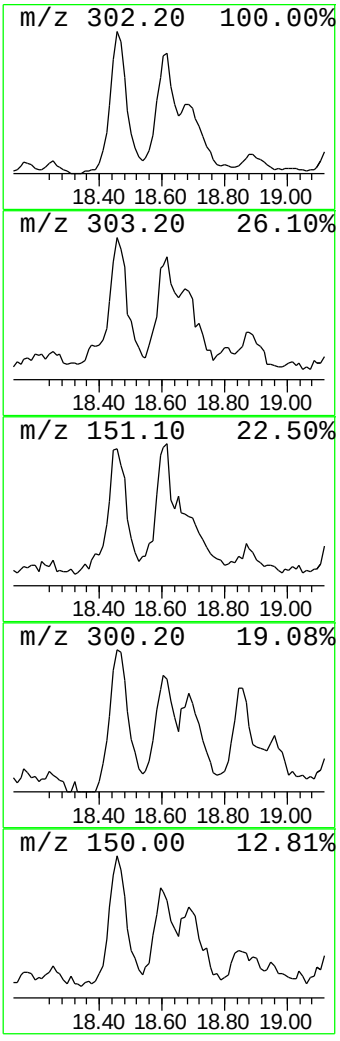
Peak Number 19 Dibenzo(a,i)pyrene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.62	2.50 ng	179554	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	95
2	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	95
3	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	89
4	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	86
5	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	76





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.72	20.4	ng	1002700	1	6.59	985512	20.0
unknown6.36	6.36	79.4	ng	3913040	1	6.59	985512	20.0
Undecane	7.22	13.2	ng	647892	1	6.59	985512	20.0
2-Tridecanone	9.56	4.9	ng	377518	3	9.63	1534950	20.0
Anthracene, 1-met...	11.62	2.3	ng	328641	4	11.10	2811130	20.0
4H-Cyclopenta[def...	11.70	2.6	ng	368587	4	11.10	2811130	20.0
Pyrene, 1-methyl-	12.86	2.1	ng	451576	5	13.71	4266690	20.0
5,12-Naphthacened...	14.40	3.8	ng	274886	6	15.06	1434730	20.0
9-Octadecenamide,...	14.49	5.0	ng	355544	6	15.06	1434730	20.0
10-Oxo-5,5-dimeth...	14.57	3.7	ng	263405	6	15.06	1434730	20.0
Benzo[e]pyrene	14.79	5.7	ng	407942	6	15.06	1434730	20.0
Benzo(a)pyrene 4,...	14.88	3.2	ng	229488	6	15.06	1434730	20.0
1,2:4,5-Dibenzopy...	18.46	3.5	ng	250450	6	15.06	1434730	20.0
Dibenzo(a,i)pyrene	18.62	2.5	ng	179554	6	15.06	1434730	20.0