LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

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-BF112916.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	5.064	240	243	252	rVB	1690513	2610505	35.66%	3.534%
2	5.476	275	279	281	rBV	5856681	6649383	90.82%	9.003%
3	6.493	365	368	371	rBV	4504650	7321451	100.00%	9.912%
4	6.630	377	380	383	rBV	5232209	6557461	89.57%	8.878%
5	6.859	398	400	403	rBV	1328295	1339565	18.30%	1.814%
6	7.019	411	414	417	rVB	4830174	4708137	64.31%	6.374%
7	7.430	446	450	452	rBV	3744425	4850167	66.25%	6.567%
8	8.150	510	513	515	rBV	1654500	1903857	26.00%	2.578%
9	9.225	604	607	610	rBV	5715628	6866094	93.78%	9.296%
10	9.613	639	641	644	rVB	432519	458199	6.26%	0.620%
11	9.899	663	666	668	rBV	2235610	2090312	28.55%	2.830%
12	10.105	677	684	685	rBV	72418	109154	1.49%	0.148%
13	10.345	698	705	706	rBV2	126255	192252	2.63%	0.260%
14	10.688	732	735	738	rBV	4240065	4770203	65.15%	6.458%
15	10.813	744	746	751	rVB	208347	248695	3.40%	0.337%
16	11.053	764	767	770	rVB	74952	119763	1.64%	0.162%
17	11.259	783	785	786	rBV	159546	125339	1.71%	0.170%
18	11.385	793	796	797	rBV	2154082	2254455	30.79%	3.052%
19	11.408	797	798	799	rVB	314745	216512	2.96%	0.293%
20	11.453	799	802	804	rBV	108132	99826	1.36%	0.135%
21	11.682	820	822	826	rVB	86334	101727	1.39%	0.138%
22	11.842	833	836	837	rBV	54907	86075	1.18%	0.117%
23	11.922	837	843	845	rVV2	828529	1457707	19.91%	1.974%
24	11.991	847	849	854	rVV2	141225	257626	3.52%	0.349%
25	12.093	854	858	861	rVV3	62762	119355	1.63%	0.162%
26	12.196	863	867	869	rVB2	76747	147396	2.01%	0.200%
27	12.425	884	887	889	rBV	64550	92154	1.26%	0.125%
28	12.505	893	894	897	rVB2	50962	74339	1.02%	0.101%
29	12.585	899	901	903	rBV	650227	725074	9.90%	0.982%
30	12.619	903	904	908	rVV4	44859	85232	1.16%	0.115%
31	12.699	908	911	918	rVV2	505742	759214	10.37%	1.028%
32	12.813	918	921	923	rVV	800528	1076810	14.71%	1.458%
33	12.871	923	926	928	rVB3	78126	131845	1.80%	0.179%
34	12.974	932	935	937	rVB	6168348	6446744	88.05%	8.728%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

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-BF112916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.145	946	950	952	rVB2	94513	184161	2.52%	0.249%
36	13.214	952	956	957	rBV2	79470	109526	1.50%	0.148%
37	13.248	957	959	960	rBV	114855	112461	1.54%	0.152%
38	13.499	979	981	984	rBV	161937	189968	2.59%	0.257%
39	13.545	984	985	991	rVB2	59574	94528	1.29%	0.128%
40	13.648	991	994	998	rVB	73521	99352	1.36%	0.135%
41	13.762	1001	1004	1005	rBV2	73863	109428	1.49%	0.148%
42	13.876	1010	1014	1022	rVB4	255233	458639	6.26%	0.621%
43	14.014	1022	1026	1031	rBV2	1847930	2525405	34.49%	3.419%
44	14.402	1055	1060	1061	rBV	63796	152328	2.08%	0.206%
45	14.425	1061	1062	1064	rVV2	54548	73733	1.01%	0.100%
46	14.494	1064	1068	1069	rVV3	60026	113835	1.55%	0.154%
47	14.517	1069	1070	1075	rVB3	62297	114072	1.56%	0.154%
48	14.802	1091	1095	1098	rVB4	31350	77863	1.06%	0.105%
49	14.871	1098	1101	1105	rVB	291249	336317	4.59%	0.455%
50	15.031	1112	1115	1120	rBV	421046	806229	11.01%	1.092%
51	15.134	1121	1124	1126	rVB2	96744	119130	1.63%	0.161%
52	15.317	1138	1140	1143	rBV	238667	313880	4.29%	0.425%
53	15.374	1143	1145	1148	rVB	208631	304344	4.16%	0.412%
54	15.442	1148	1151	1154	rBV	1001730	1316313	17.98%	1.782%
55	15.911	1190	1192	1196	rBV2	34924	81086	1.11%	0.110%
56	16.414	1231	1236	1239	rBV2	39805	117793	1.61%	0.159%
57	16.677	1253	1259	1265	rBV4	43535	142564	1.95%	0.193%
58	16.837	1269	1273	1277	rVV2	131130	262271	3.58%	0.355%
59	17.008	1282	1288	1290	rVV2	24597	82616	1.13%	0.112%
60	17.065	1290	1293	1300	rVB3	36471	112823	1.54%	0.153%
61	17.248	1306	1309	1319	rVB	116760	269632	3.68%	0.365%
62	19.397	1490	1497	1505	rVB4	28728	127876	1.75%	0.173%

Sum of corrected areas: 73860801

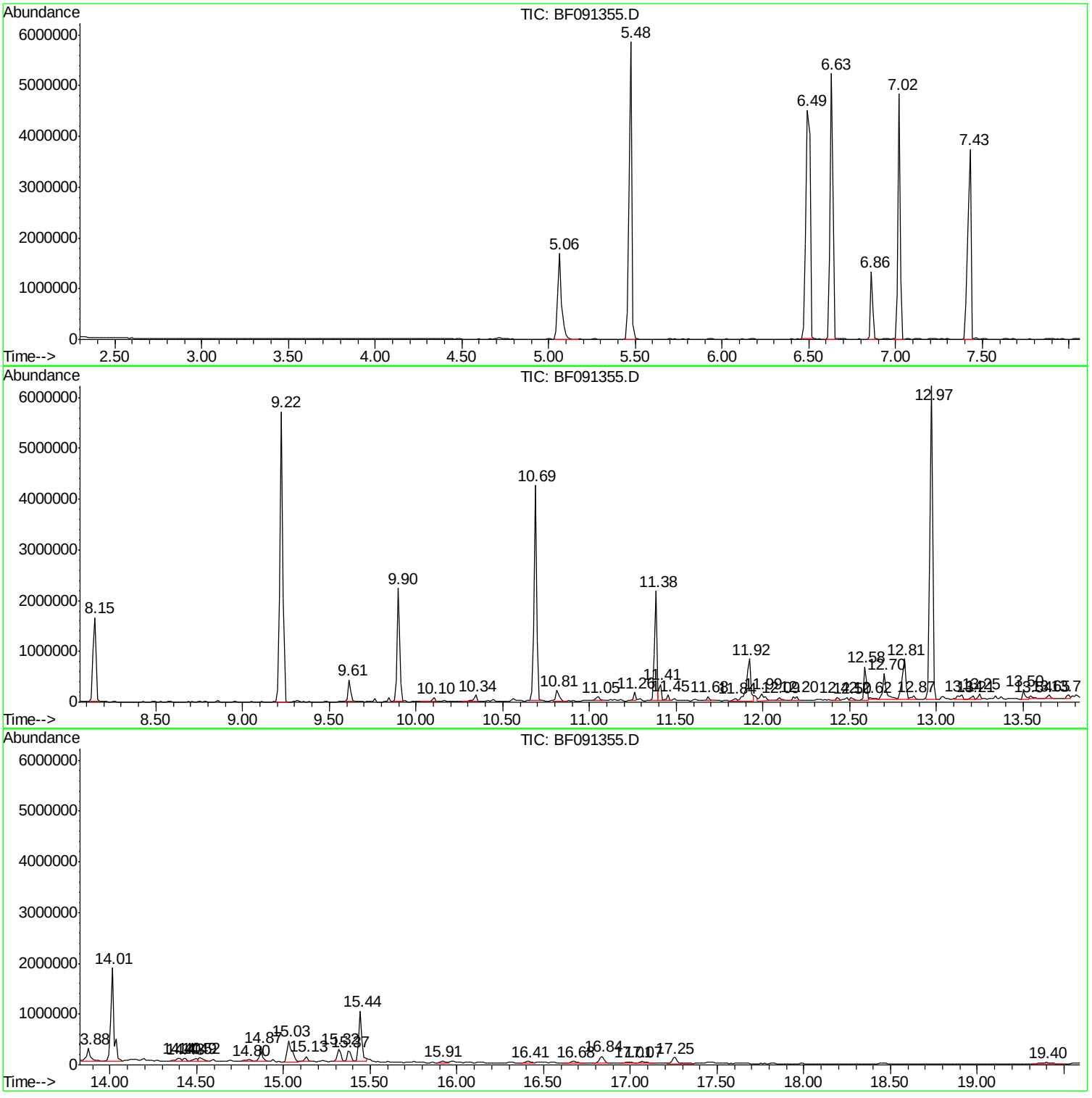
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

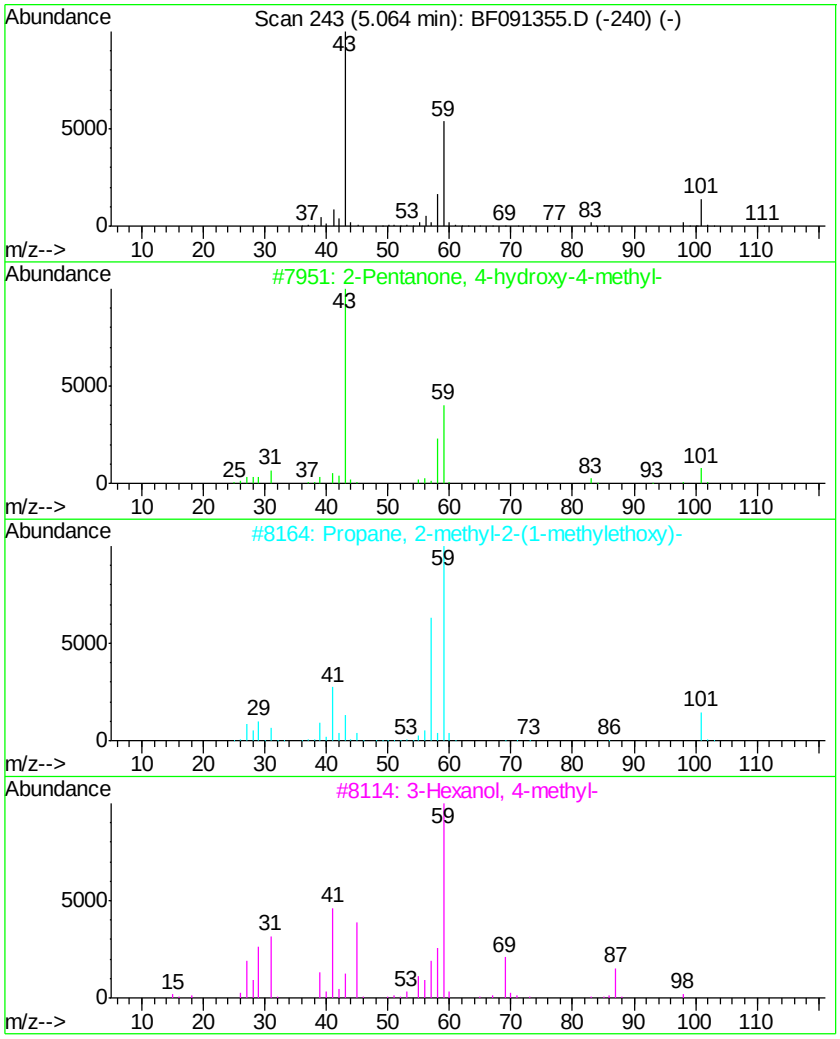
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

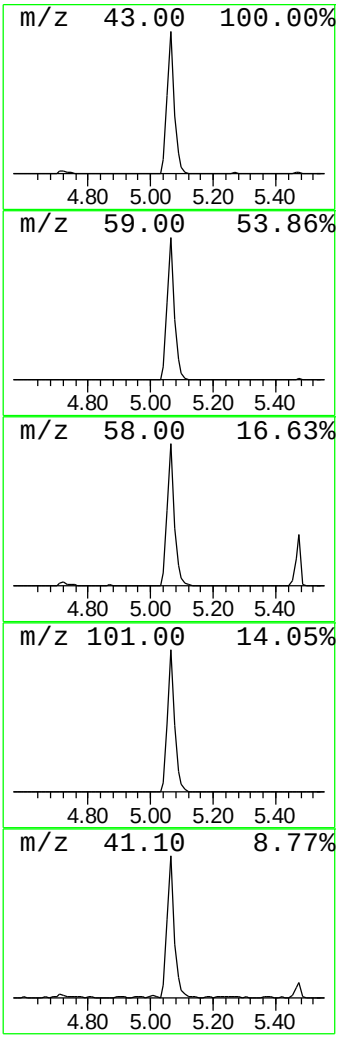
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	38.98 ng	2610510	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

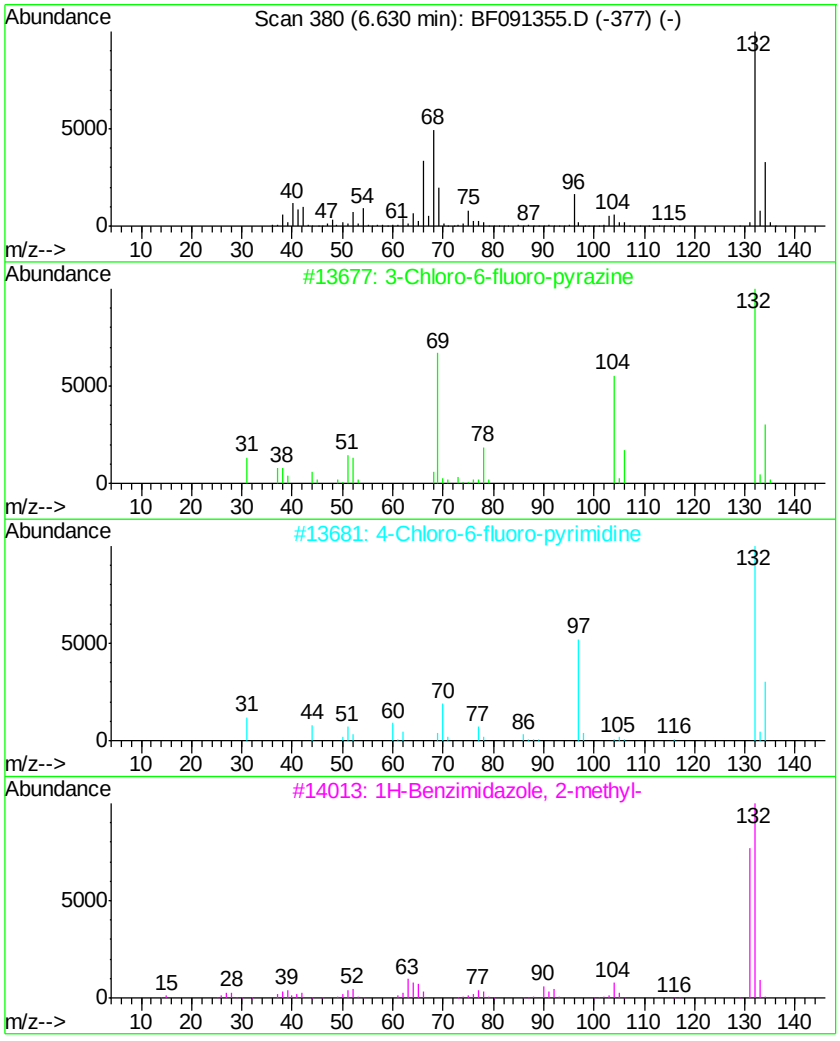
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

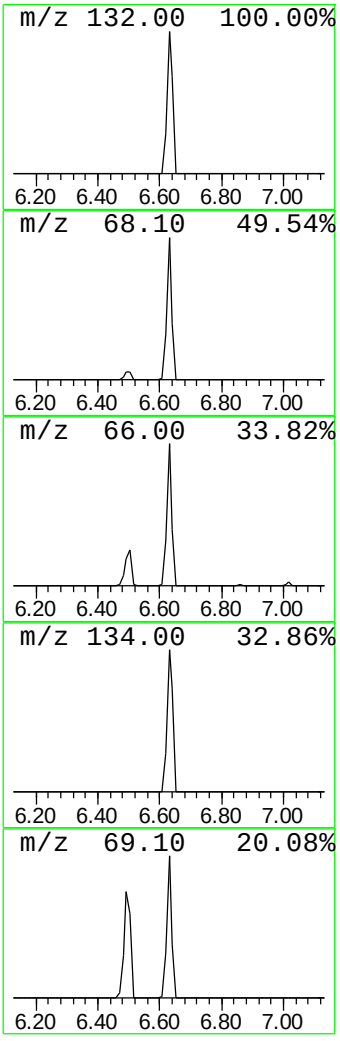
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	97.90 ng	6557460	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

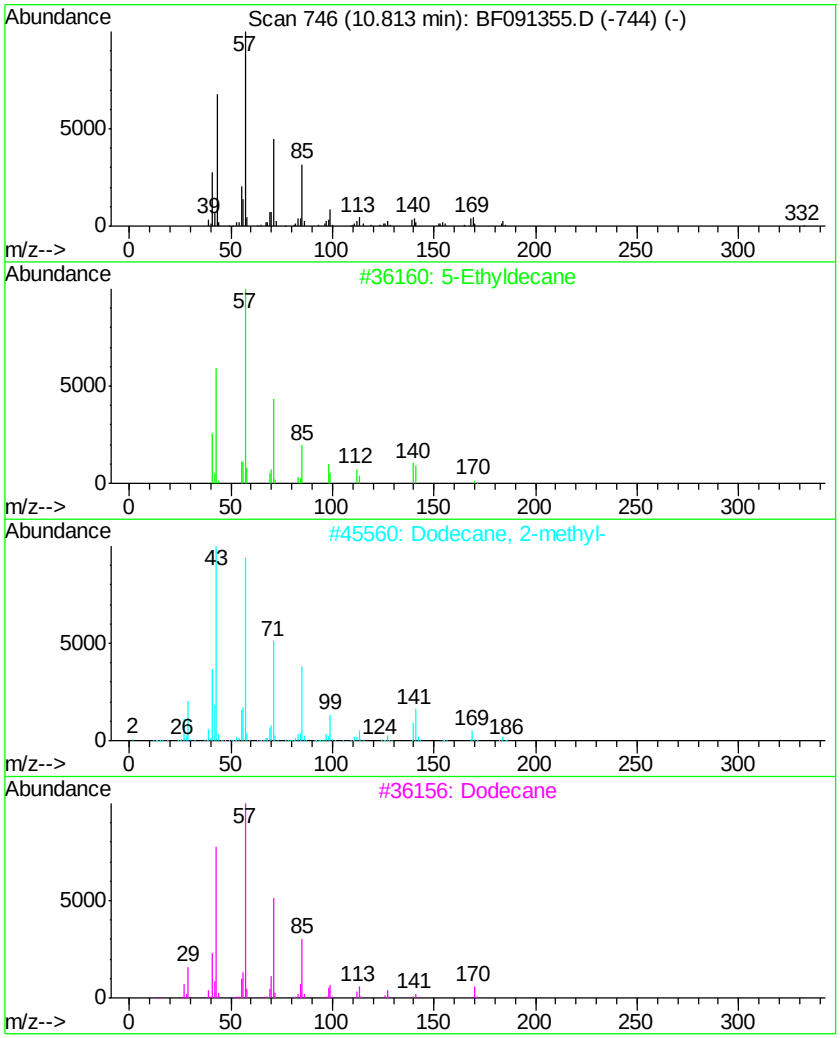
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

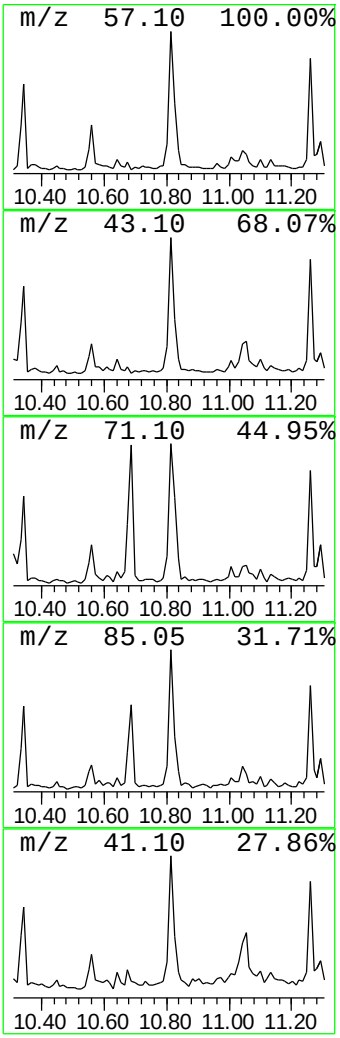
****

Peak Number 4 5-Ethyldecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.21 ng	248695	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyldecane	170	C12H26	017302-36-2	80
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
3	Dodecane	170	C12H26	000112-40-3	80
4	Tridecane	184	C13H28	000629-50-5	80
5	Hexadecane	226	C16H34	000544-76-3	74





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

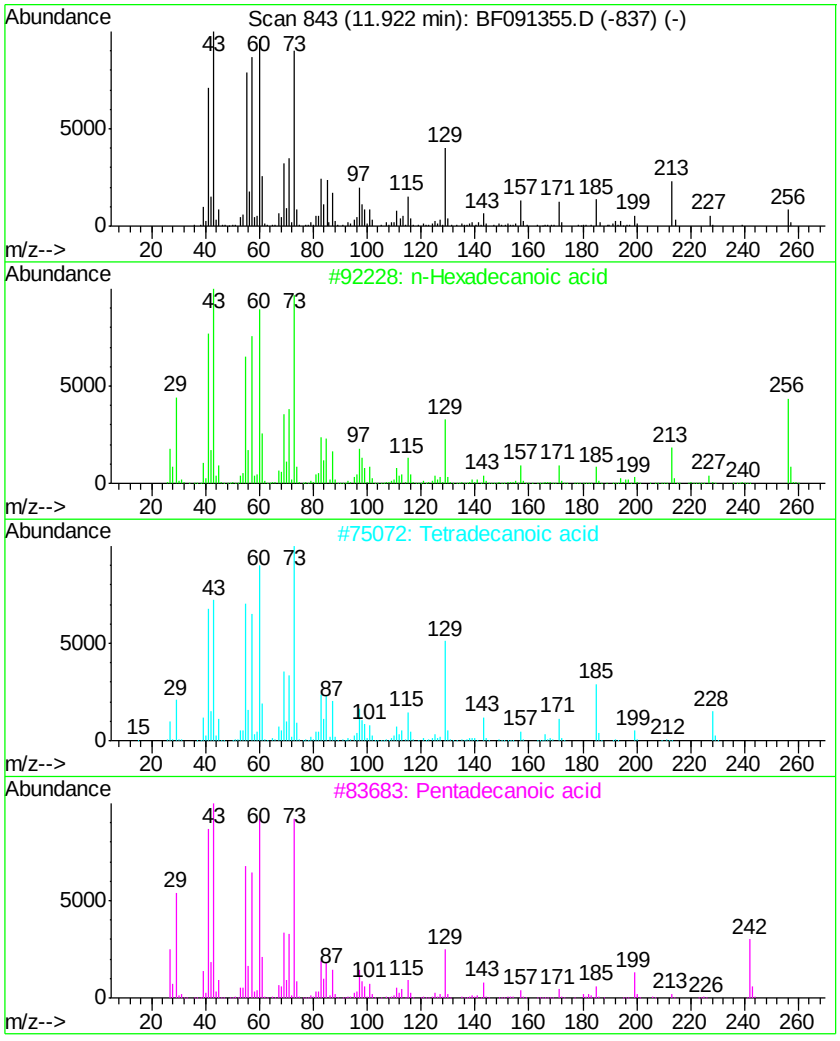
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

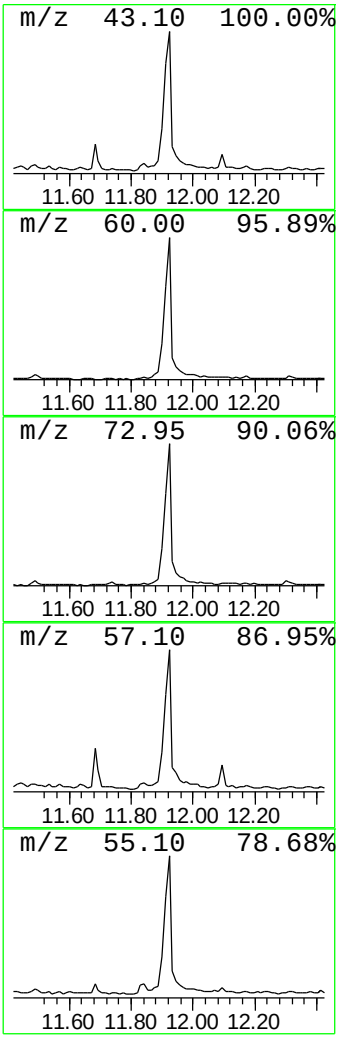
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	12.93 ng	1457710	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

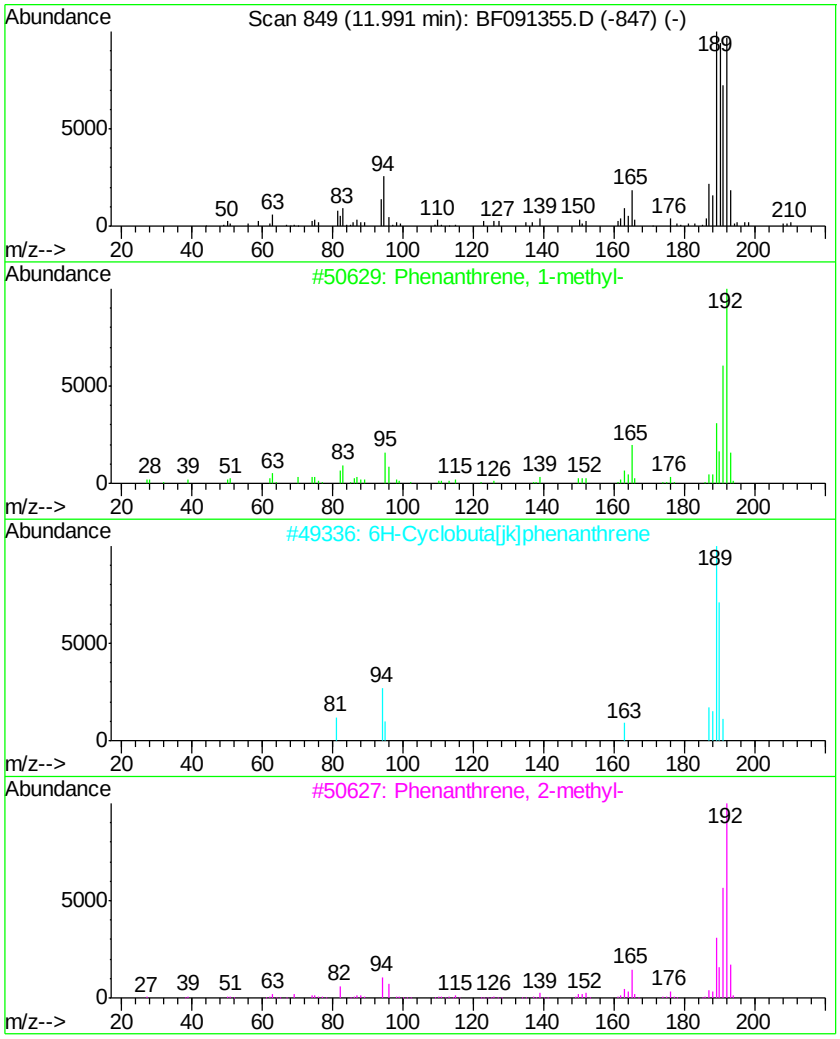
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

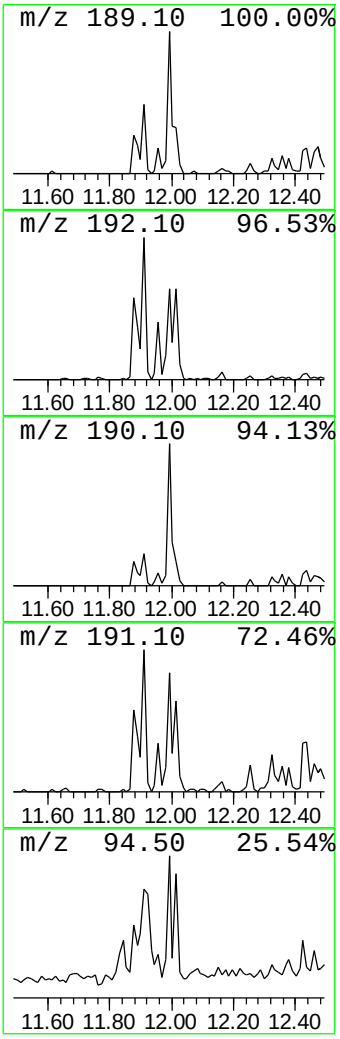
****

Peak Number 6 Phenanthrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.29 ng	257626	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	55
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

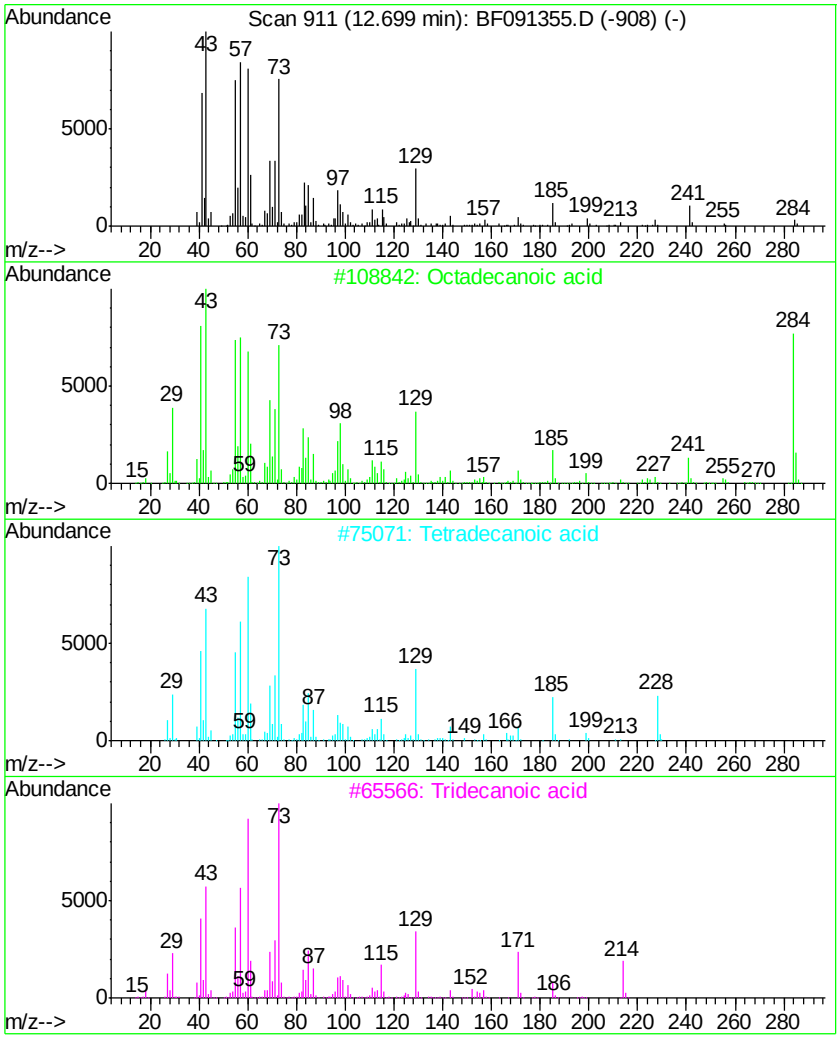
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

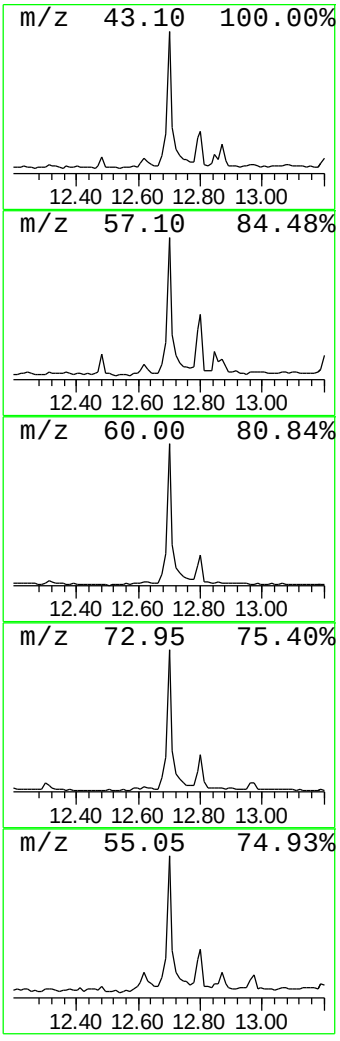
****

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	6.01 ng	759214	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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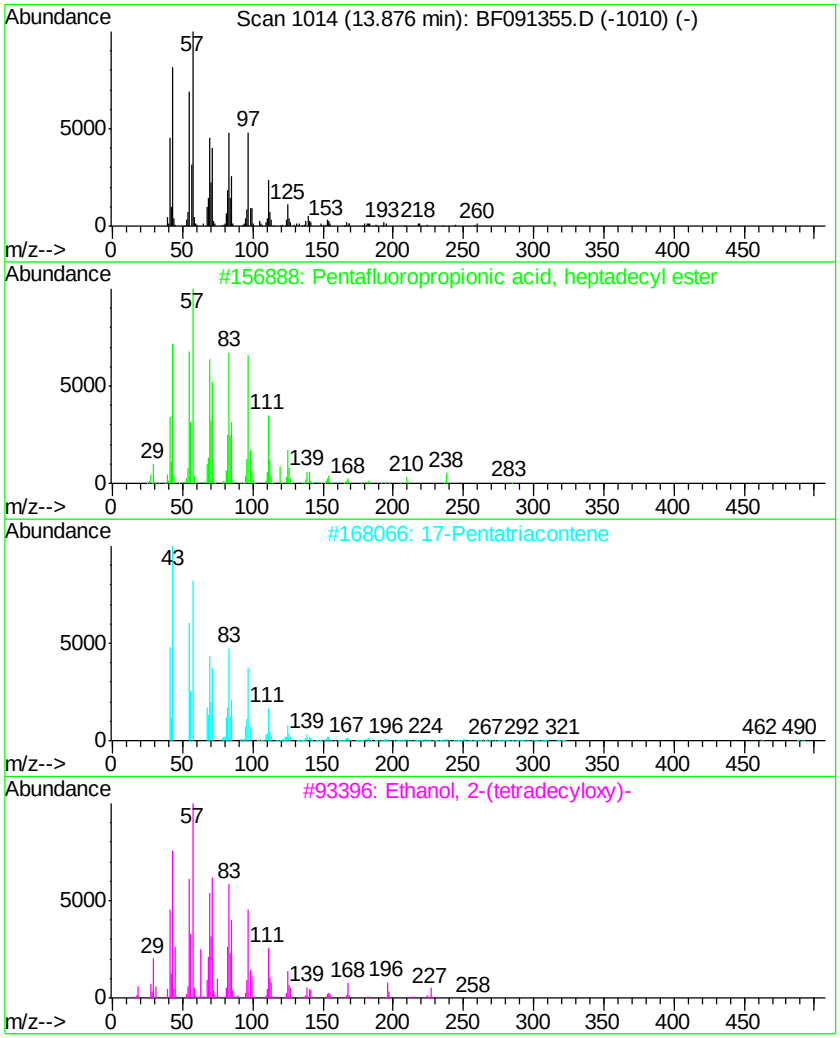
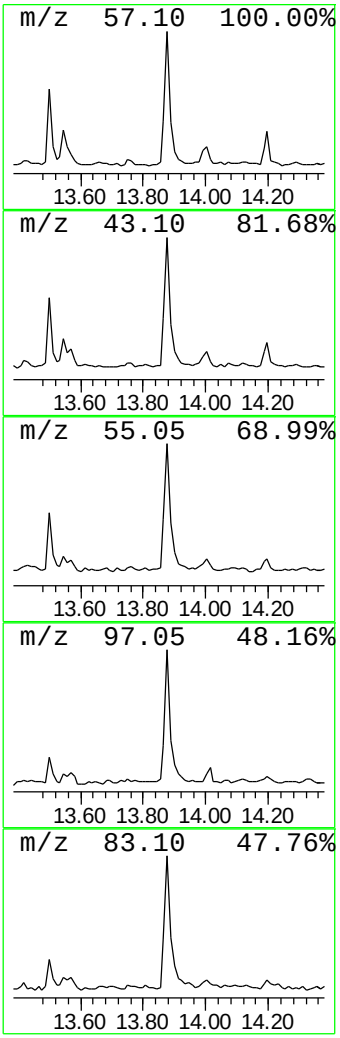
Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.63 ng	458639	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	81
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	74





Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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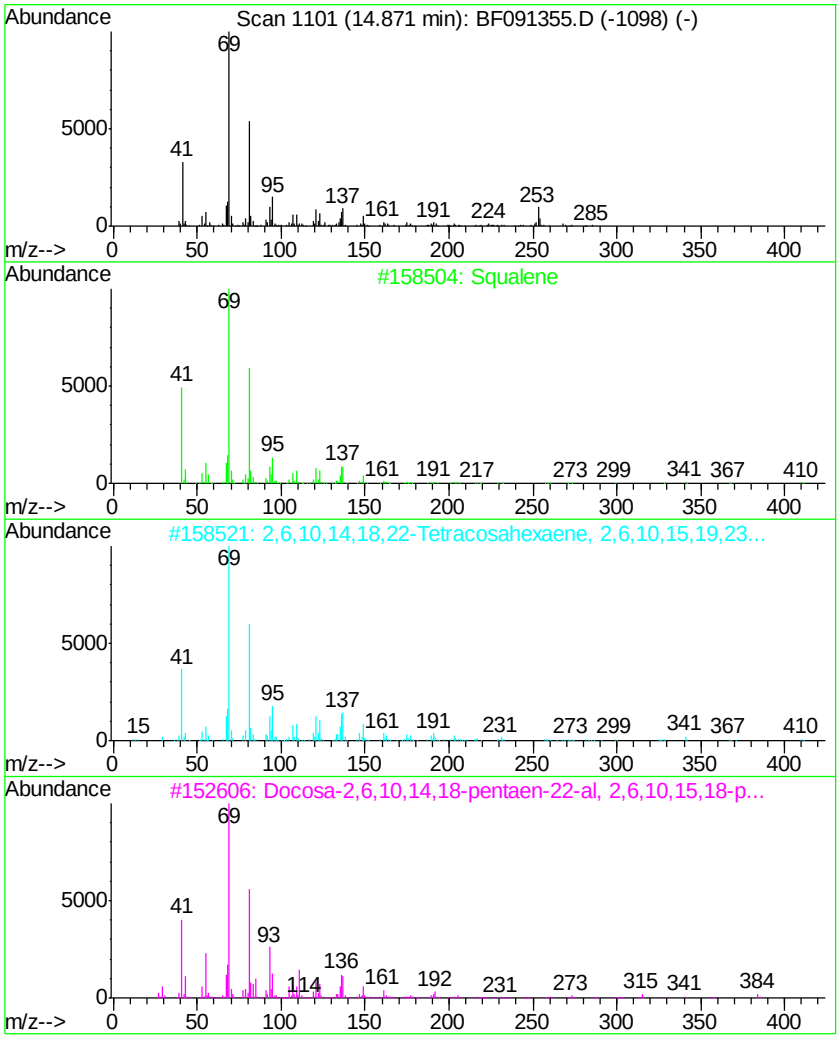
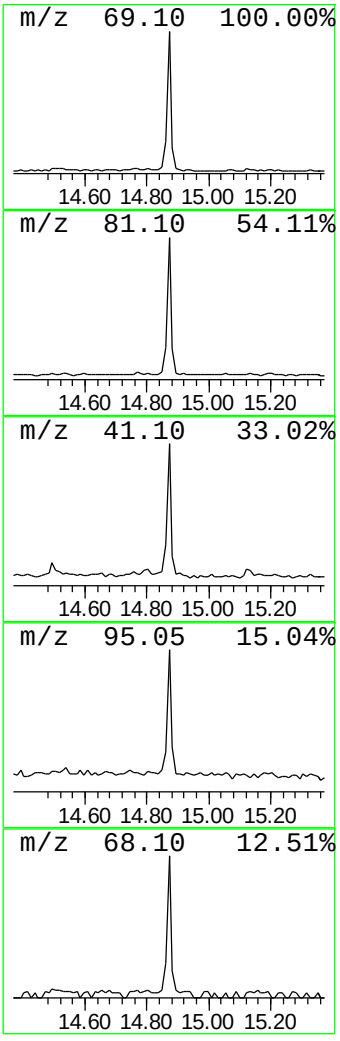
Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	5.11 ng	336317	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	76
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	74
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4	Farnesol isomer a	222	C15H26O	1000108-92-4	59
5	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	59





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Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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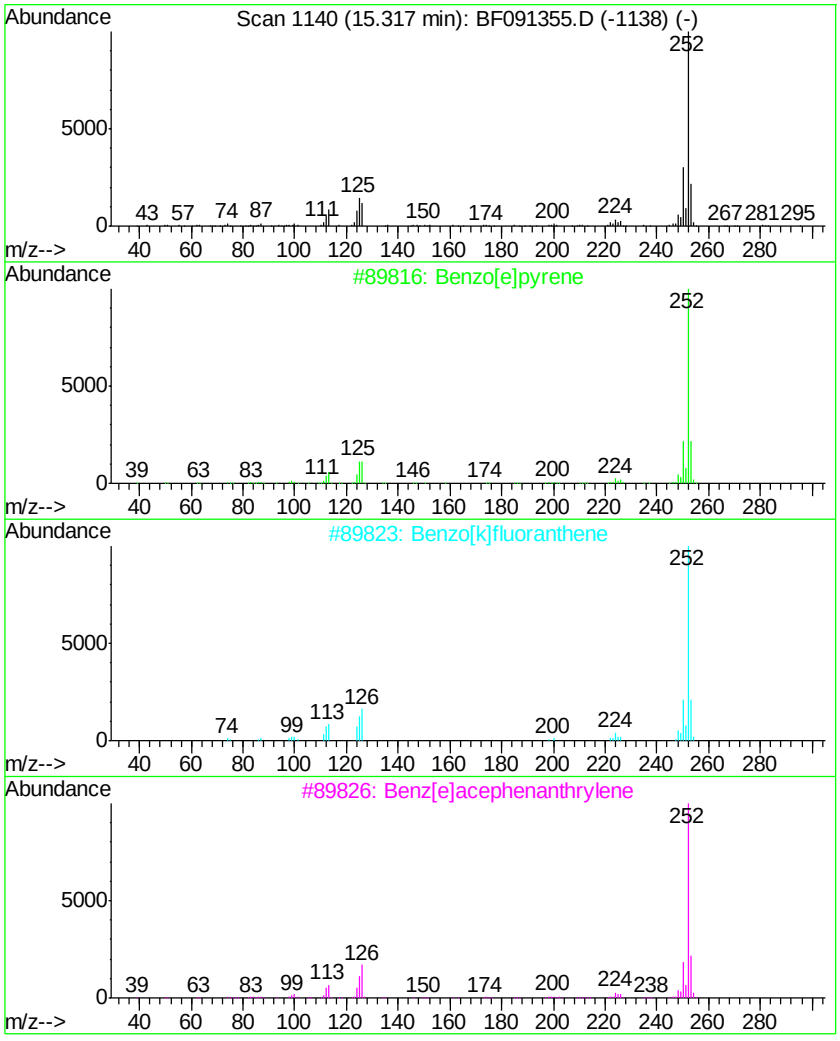
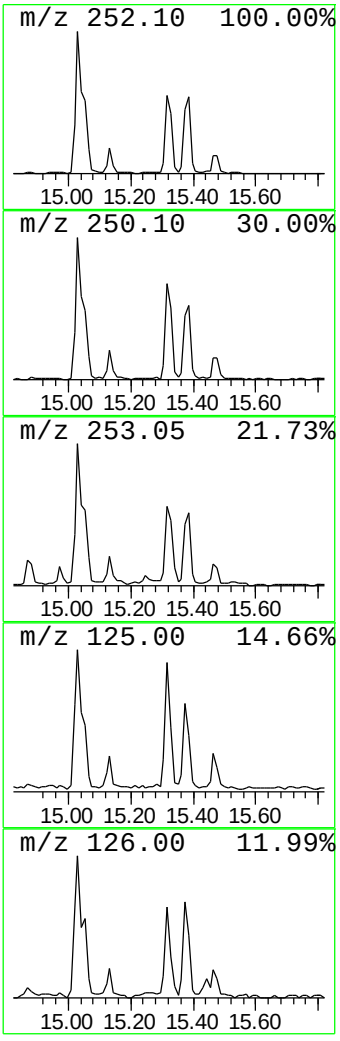
Peak Number 10 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	4.77 ng	313880	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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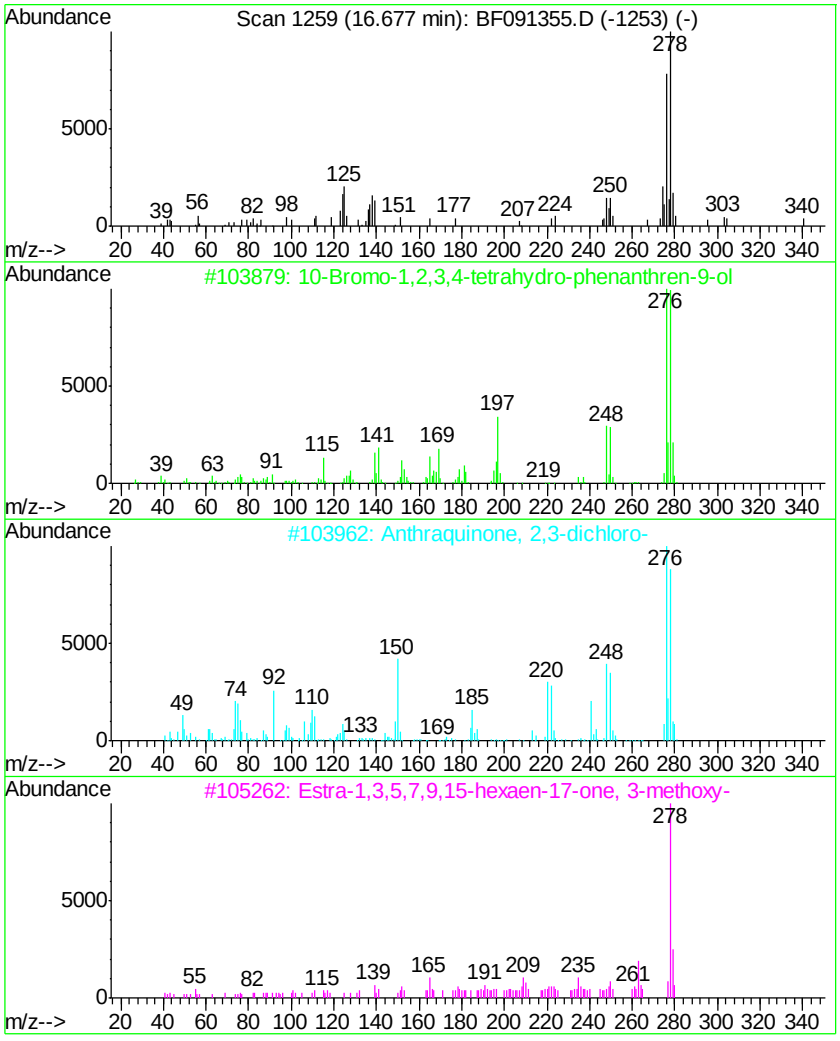
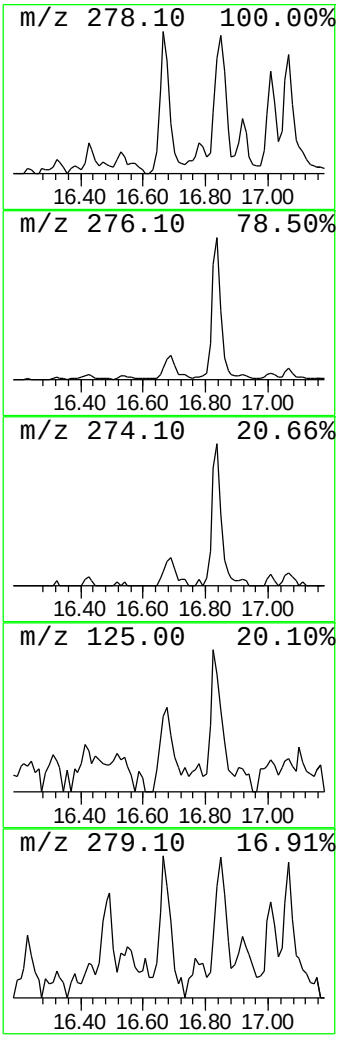
Peak Number 11 10-Bromo-1,2,3,4-tetrahydro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.68	2.17 ng	142564	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Bromo-1,2,3,4-tetrahydro-phen...	276	C14H13BrO	1000190-54-9	64
2	Anthraquinone, 2,3-dichloro-	276	C14H6Cl2O2	000084-45-7	50
3	Estra-1,3,5,7,9,15-hexaen-17-one...	278	C19H18O2	056588-53-5	38
4	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	38
5	Oxazolo[5',4':4,5]pyrido[2,3-d]p...	276	C12H12N4O4	349496-92-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091355.D
Acq On : 30 Nov 2016 15:37
Operator : UM/SJ
Sample : H5749-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	39.0	ng	2610510	1	6.86	1339570	20.0
unknown6.63	6.63	97.9	ng	6557460	1	6.86	1339570	20.0
5-Ethyldecane	10.81	2.2	ng	248695	4	11.38	2254460	20.0
n-Hexadecanoic acid	11.92	12.9	ng	1457710	4	11.38	2254460	20.0
Phenanthrene, 1-m...	11.99	2.3	ng	257626	4	11.38	2254460	20.0
Octadecanoic acid	12.70	6.0	ng	759214	5	14.01	2525410	20.0
Pentafluoropropio...	13.88	3.6	ng	458639	5	14.01	2525410	20.0
Squalene	14.87	5.1	ng	336317	6	15.44	1316310	20.0
Benzo[e]pyrene	15.32	4.8	ng	313880	6	15.44	1316310	20.0
10-Bromo-1,2,3,4-...	16.68	2.2	ng	142564	6	15.44	1316310	20.0