LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096357.D
Acq On : 1 Jul 2017 1:00
Operator : SJ/MA
Sample : I3930-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-6-8

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-BF062717.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	4.963	484	489	499	rVB	469384	650837	16.73%	1.762%
2	5.381	554	560	563	rVB	3732282	3888977	99.98%	10.529%
3	5.704	612	615	621	rVB	43663	39290	1.01%	0.106%
4	6.392	727	732	735	rBV	3468172	3889803	100.00%	10.531%
5	6.528	750	755	759	rBV	3584444	3667860	94.29%	9.930%
6	6.757	790	794	798	rBV	1134836	947689	24.36%	2.566%
7	6.916	817	821	824	rBV	2965479	2695794	69.30%	7.299%
8	7.316	884	889	892	rBV	2324895	2338520	60.12%	6.331%
9	7.404	901	904	909	rVB2	48914	49990	1.29%	0.135%
10	8.039	1007	1012	1015	rBV	1435075	1258436	32.35%	3.407%
11	8.751	1128	1133	1136	rVB	64549	55340	1.42%	0.150%
12	8.851	1147	1150	1153	rBV	50894	40538	1.04%	0.110%
13	9.116	1190	1195	1198	rBV	3144623	2937010	75.51%	7.952%
14	9.210	1208	1211	1215	rVB2	55452	53120	1.37%	0.144%
15	9.451	1245	1252	1255	rBV	50063	60518	1.56%	0.164%
16	9.510	1258	1262	1264	rVV	487925	424060	10.90%	1.148%
17	9.651	1282	1286	1289	rBV	53706	39501	1.02%	0.107%
18	9.739	1298	1301	1305	rVB	91031	72838	1.87%	0.197%
19	9.792	1305	1310	1313	rBV	1203462	1026954	26.40%	2.780%
20	9.822	1313	1315	1318	rVB	78803	64740	1.66%	0.175%
21	9.998	1342	1345	1348	rVB	85597	73664	1.89%	0.199%
22	10.233	1383	1385	1389	rVB	104513	87617	2.25%	0.237%
23	10.339	1400	1403	1406	rBV	70355	66006	1.70%	0.179%
24	10.457	1419	1423	1427	rBV	32177	42961	1.10%	0.116%
25	10.575	1439	1443	1447	rBV	1729958	1615140	41.52%	4.373%
26	10.710	1462	1466	1473	rVB	113155	141169	3.63%	0.382%
27	11.075	1525	1528	1533	rVB	39199	44027	1.13%	0.119%
28	11.157	1539	1542	1546	rBV2	52973	58815	1.51%	0.159%
29	11.269	1558	1561	1564	rBV	861575	876307	22.53%	2.373%
30	11.292	1564	1565	1569	rVV	574536	449882	11.57%	1.218%
31	11.345	1569	1574	1577	rVB	174147	151741	3.90%	0.411%
32	11.498	1595	1600	1604	rBV2	61668	73467	1.89%	0.199%
33	11.774	1644	1647	1649	rBV2	81707	66386	1.71%	0.180%
34	11.810	1649	1653	1655	rVV2	315818	339900	8.74%	0.920%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3930-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-6-8

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-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.839	1655	1658	1662	rVV2	102570	133327	3.43%	0.361%
36	11.880	1662	1665	1668	rVV	118863	143492	3.69%	0.388%
37	11.904	1668	1669	1674	rVB	58240	42518	1.09%	0.115%
38	12.069	1694	1697	1698	rBV2	68984	59404	1.53%	0.161%
39	12.321	1736	1740	1743	rBV2	65255	72707	1.87%	0.197%
40	12.404	1751	1754	1760	rVB3	43303	60693	1.56%	0.164%
41	12.480	1763	1767	1770	rBV	764940	628126	16.15%	1.701%
42	12.592	1781	1786	1790	rBV3	67733	92354	2.37%	0.250%
43	12.710	1798	1806	1809	rBV2	571029	709952	18.25%	1.922%
44	12.857	1827	1831	1834	rVV	2335282	2132145	54.81%	5.773%
45	12.886	1834	1836	1839	rVB	54049	40694	1.05%	0.110%
46	12.927	1839	1843	1846	rBV2	51002	67666	1.74%	0.183%
47	13.033	1859	1861	1864	rVB	89865	92373	2.37%	0.250%
48	13.104	1870	1873	1875	rVB	74385	71373	1.83%	0.193%
49	13.139	1875	1879	1882	rBV2	92636	101379	2.61%	0.274%
50	13.263	1897	1900	1904	rBV2	48417	45357	1.17%	0.123%
51	13.339	1908	1913	1921	rVB	788797	736660	18.94%	1.994%
52	13.404	1921	1924	1928	rBV2	128914	143210	3.68%	0.388%
53	13.539	1944	1947	1949	rBV	52368	46474	1.19%	0.126%
54	13.651	1962	1966	1969	rBV2	70211	105171	2.70%	0.285%
55	13.704	1973	1975	1979	rVV2	51934	66180	1.70%	0.179%
56	13.757	1979	1984	1989	rVV3	247572	295209	7.59%	0.799%
57	13.904	2004	2009	2011	rBV2	980795	1194726	30.71%	3.235%
58	13.927	2011	2013	2016	rVB	294398	217837	5.60%	0.590%
59	14.010	2024	2027	2033	rBV4	37821	66846	1.72%	0.181%
60	14.086	2038	2040	2043	rVB	49990	44288	1.14%	0.120%
61	14.915	2177	2181	2190	rBV	218694	393031	10.10%	1.064%
62	15.204	2227	2230	2235	rVB	136222	159258	4.09%	0.431%
63	15.257	2236	2239	2243	rVB	147120	172683	4.44%	0.468%
64	15.321	2246	2250	2253	rBV	464003	511728	13.16%	1.385%

Sum of corrected areas: 36935758

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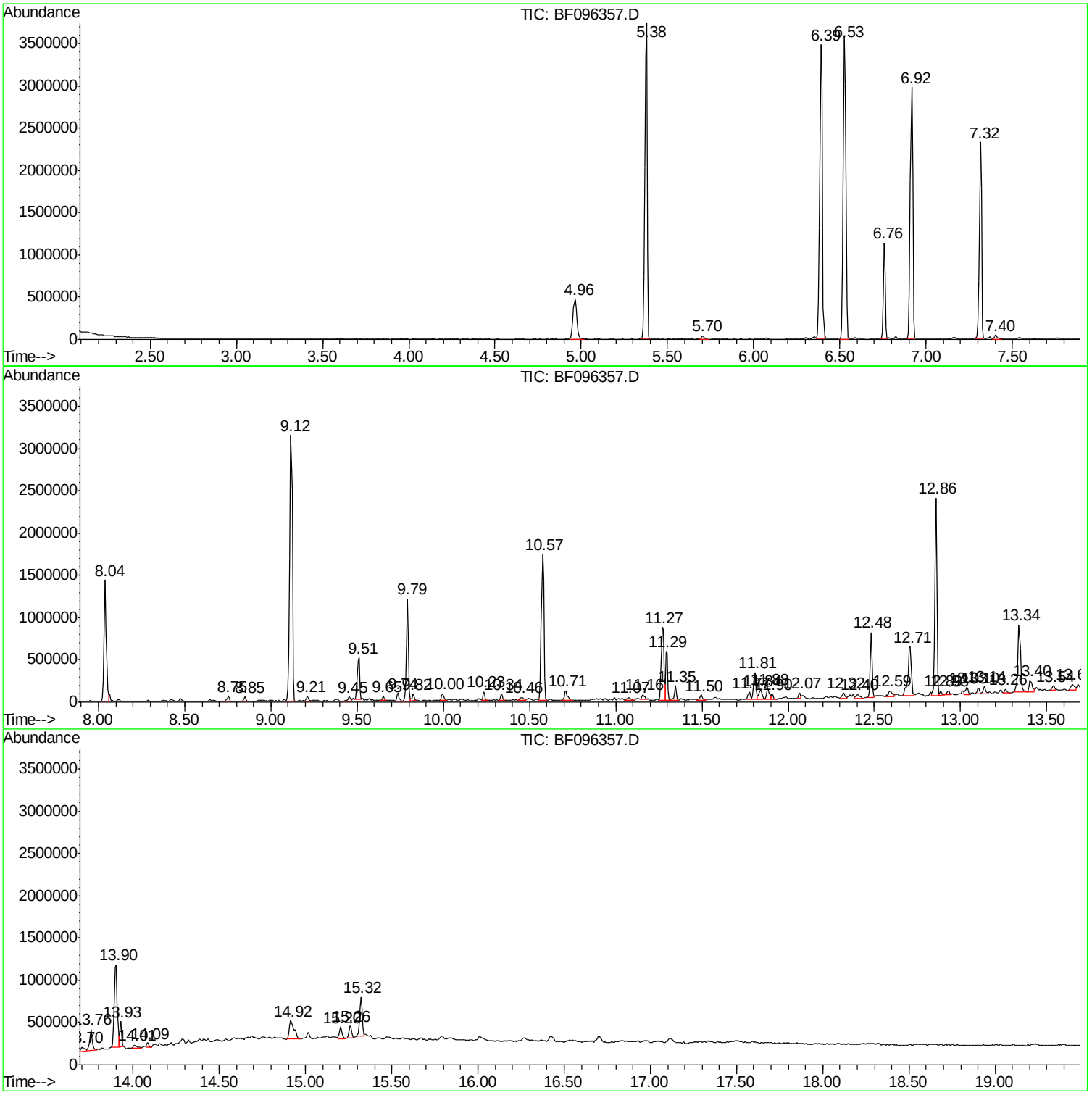
Instrument :
BNA_F
ClientSampleId :
B2-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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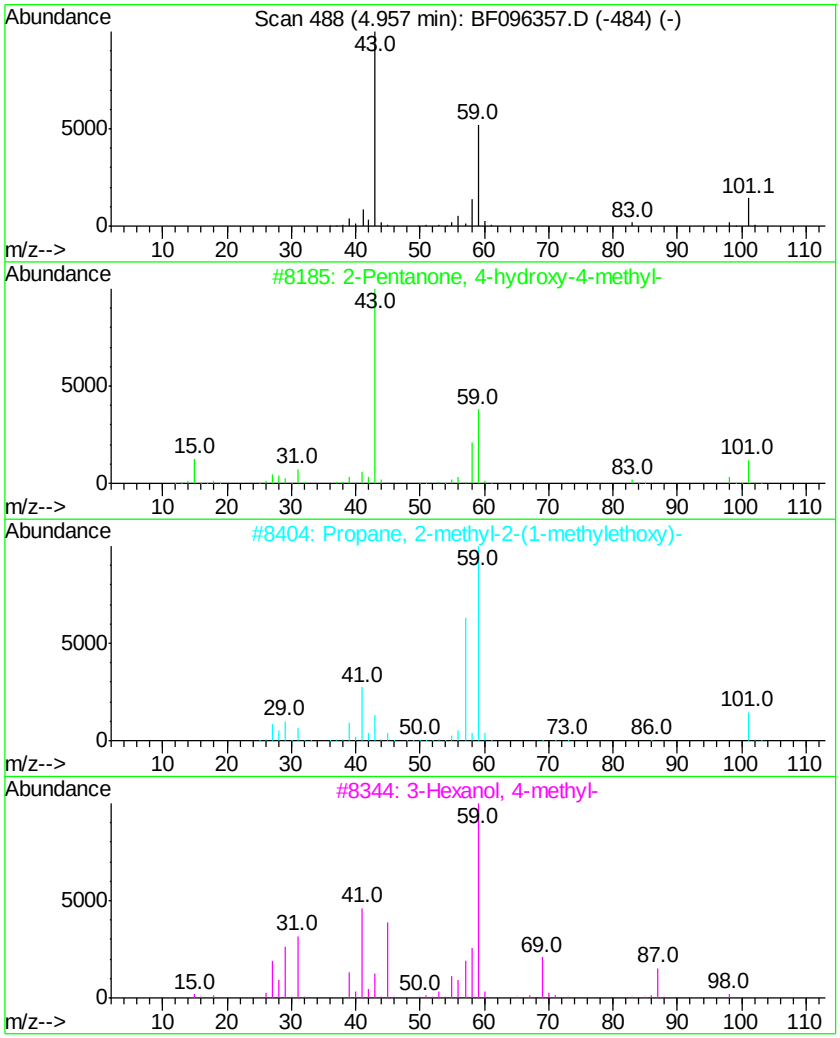
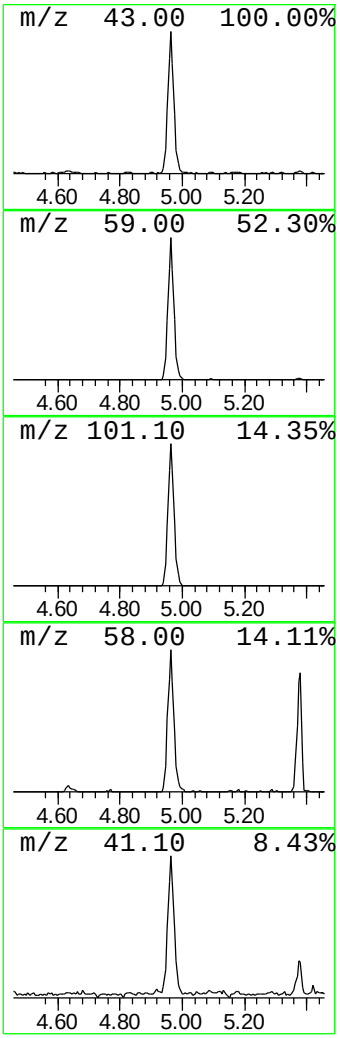
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	13.74 ng	650837	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
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	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : I3930-04
Misc :
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Instrument : BNA_F
ClientSampleId : B2-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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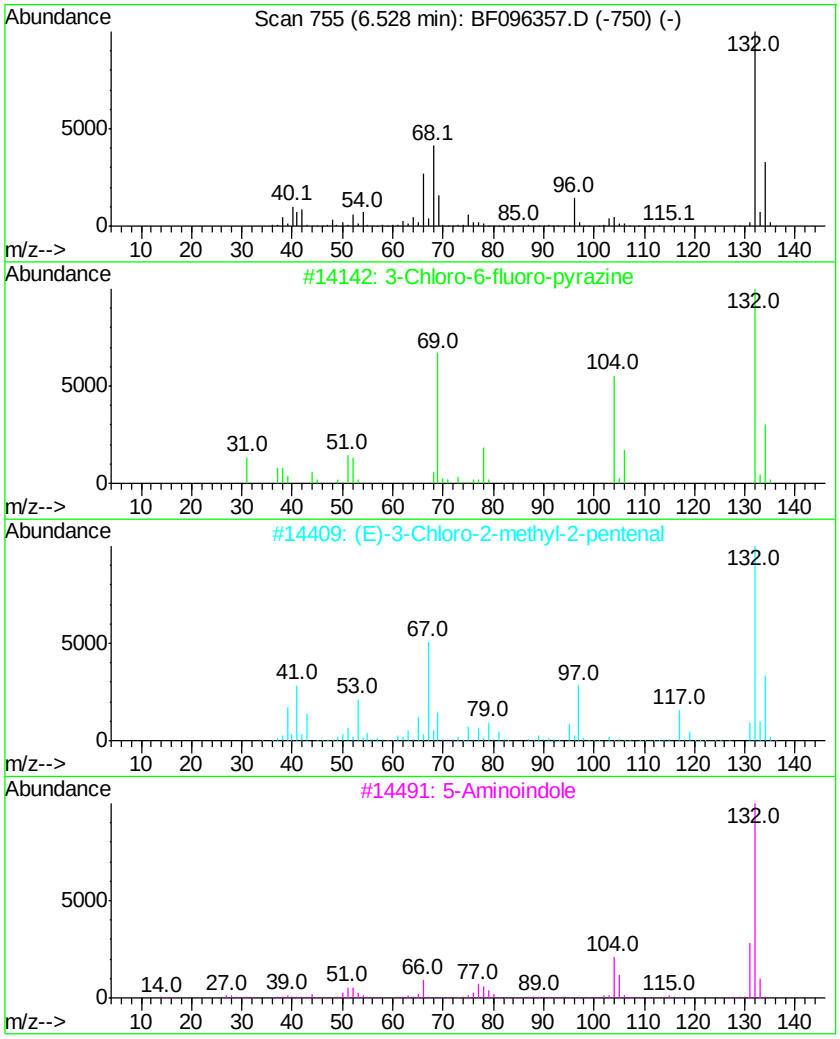
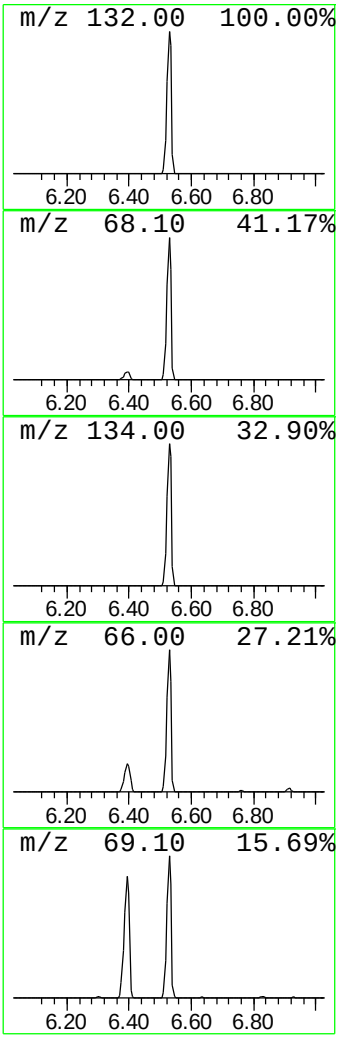
Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	77.41 ng	3667860	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : I3930-04
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Instrument : BNA_F
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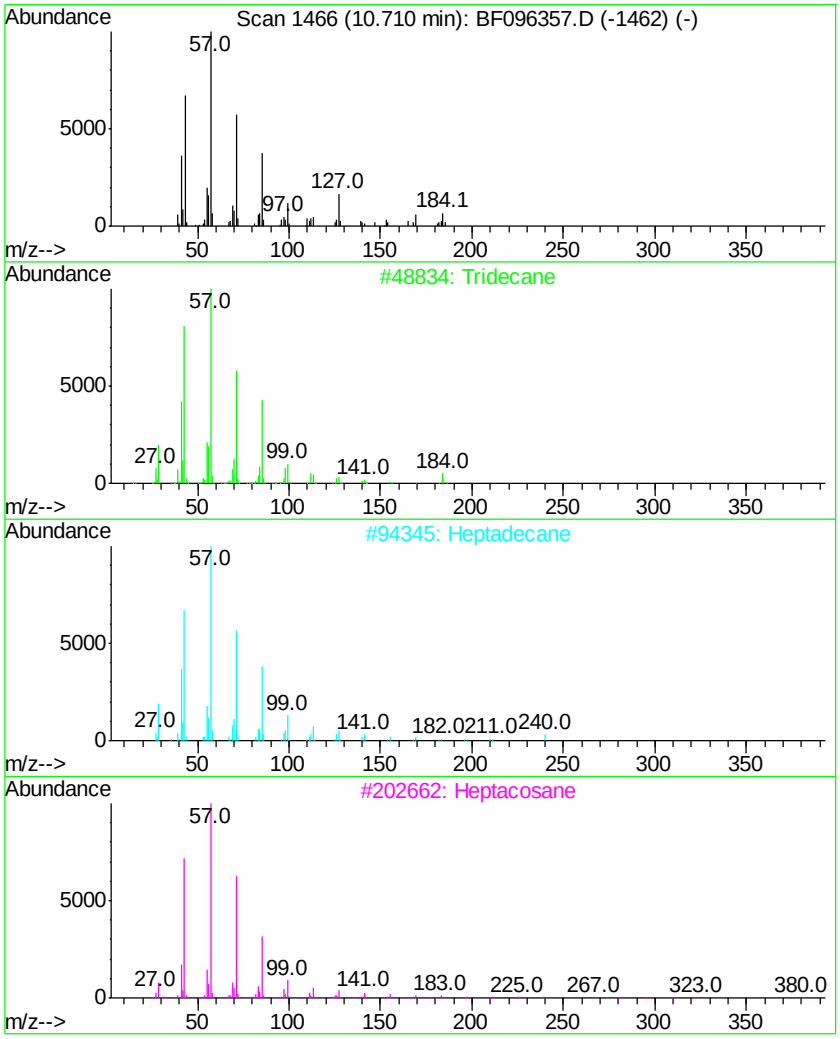
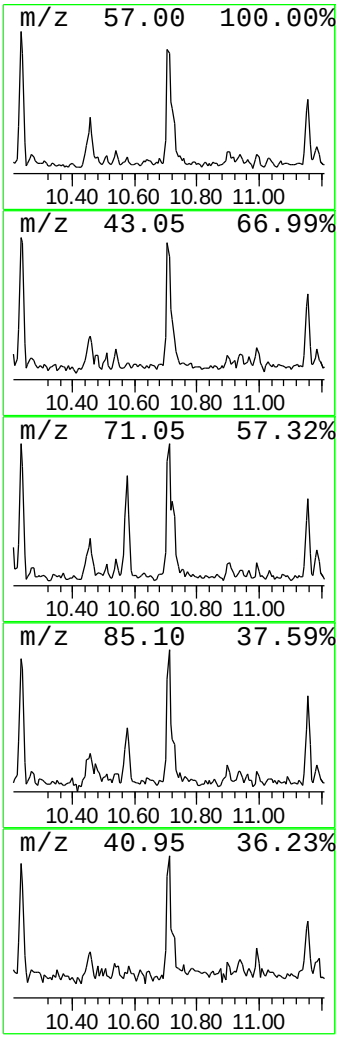
Peak Number 4 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	3.22 ng	141169	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Heptadecane	240	C17H36	000629-78-7	86
3	Heptacosane	380	C27H56	000593-49-7	72
4	Tetracosane	338	C24H50	000646-31-1	72
5	Eicosane	282	C20H42	000112-95-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
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Instrument : BNA_F
ClientSampleId : B2-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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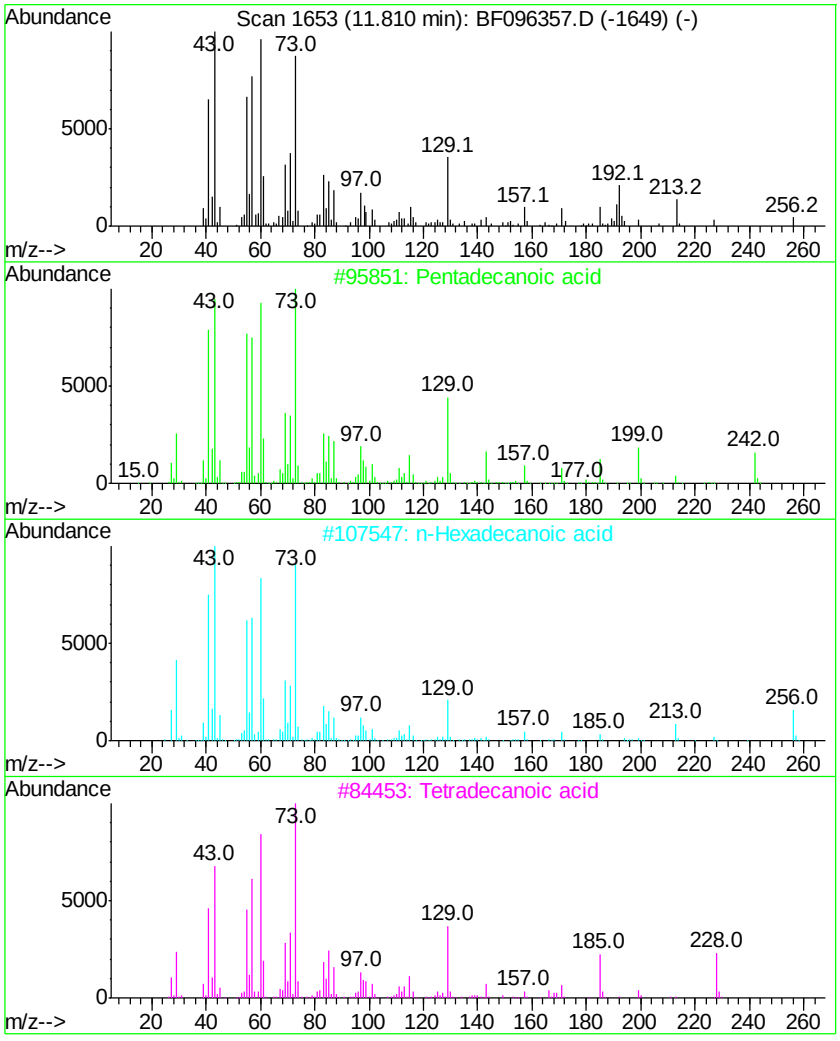
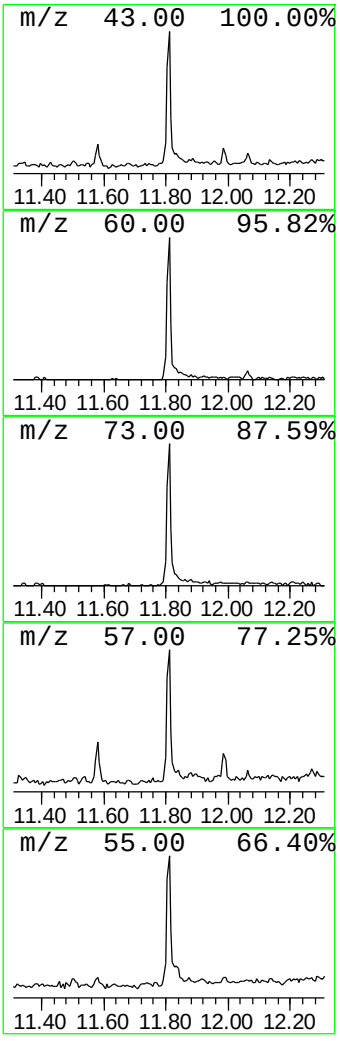
Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	7.76 ng	339900	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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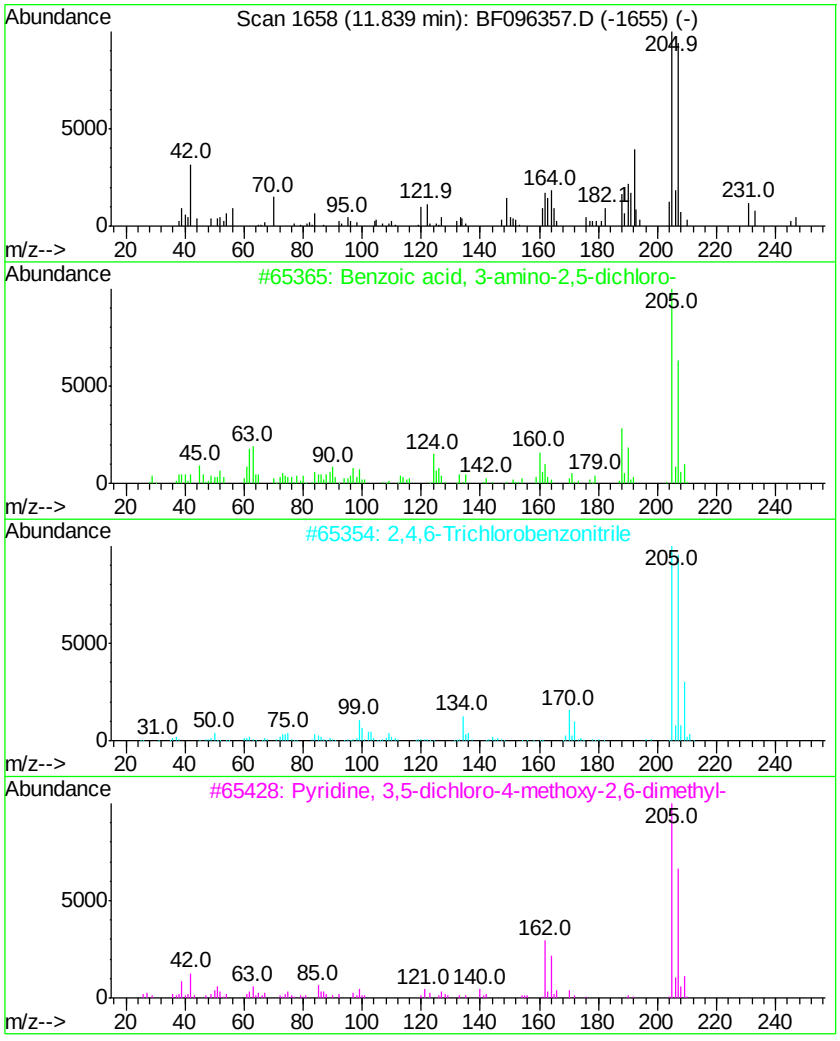
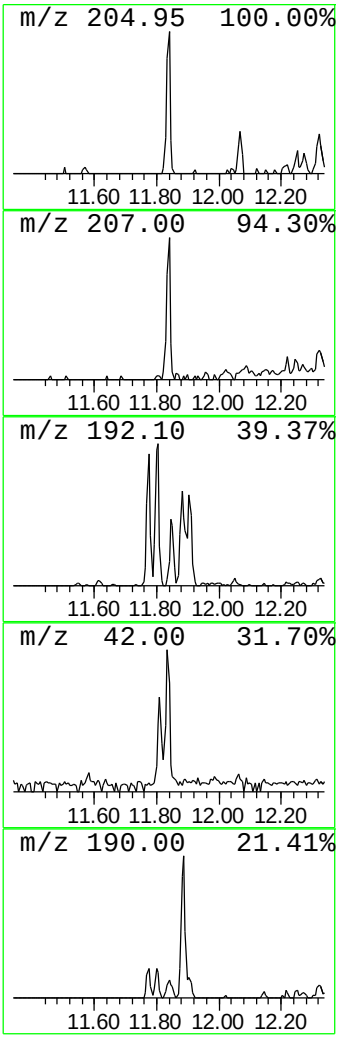
Peak Number 6 Benzoic acid, 3-amino-2,5-d... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.04 ng	133327	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	64
2	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	52
3	Pyridine, 3,5-dichloro-4-methoxy...	205	C8H9Cl2NO	051050-42-1	50
4	Benzenamine, 4-bromo-2-chloro-	205	C6H5BrClN	038762-41-3	50
5	2-Bromo-4-chloroaniline	205	C6H5BrClN	000873-38-1	50





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

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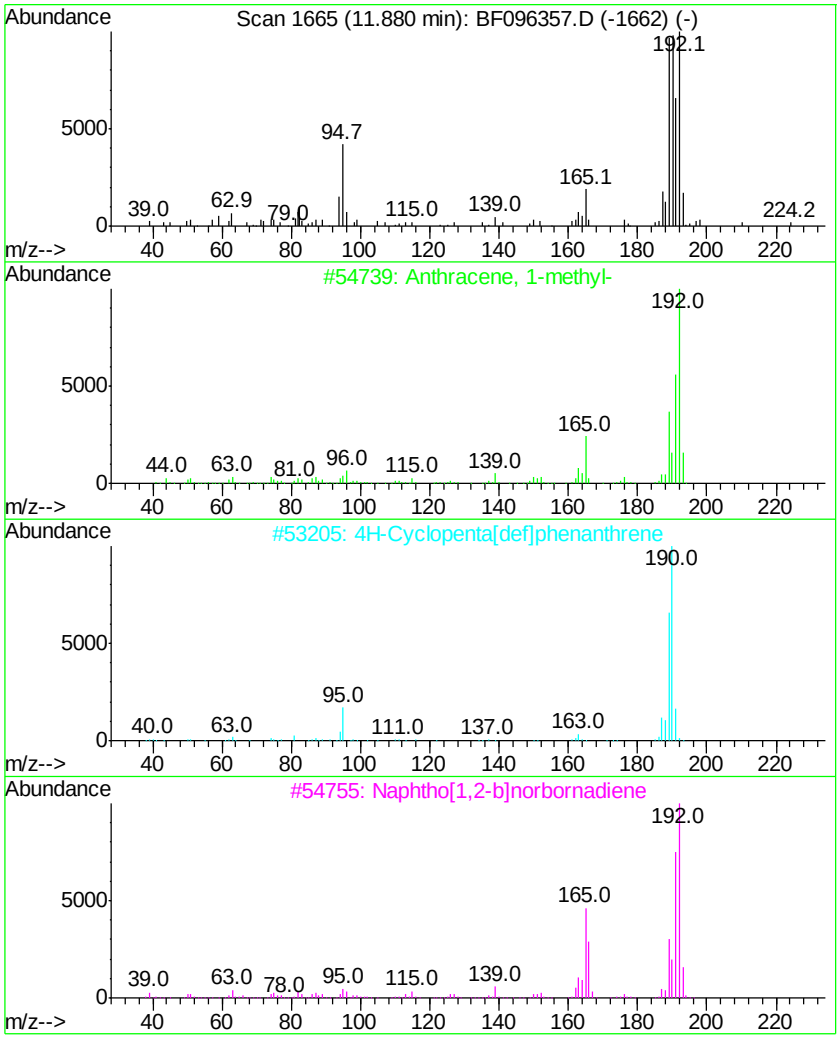
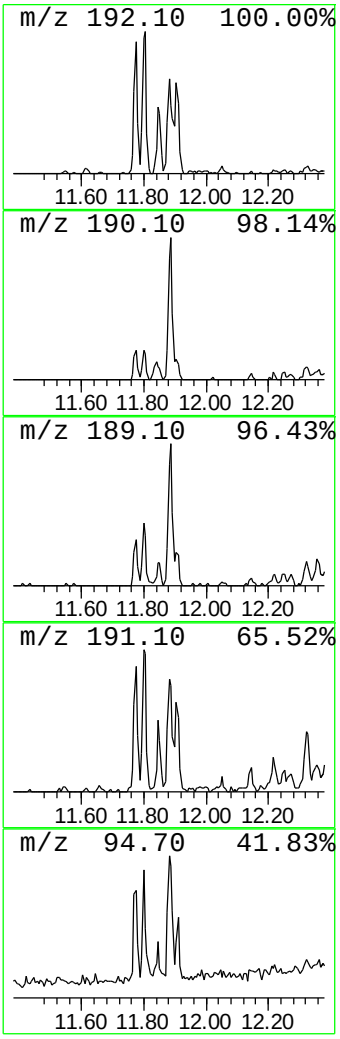
Peak Number 7 Anthracene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.27 ng	143492	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	80
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	50
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	47
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46





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Sample : I3930-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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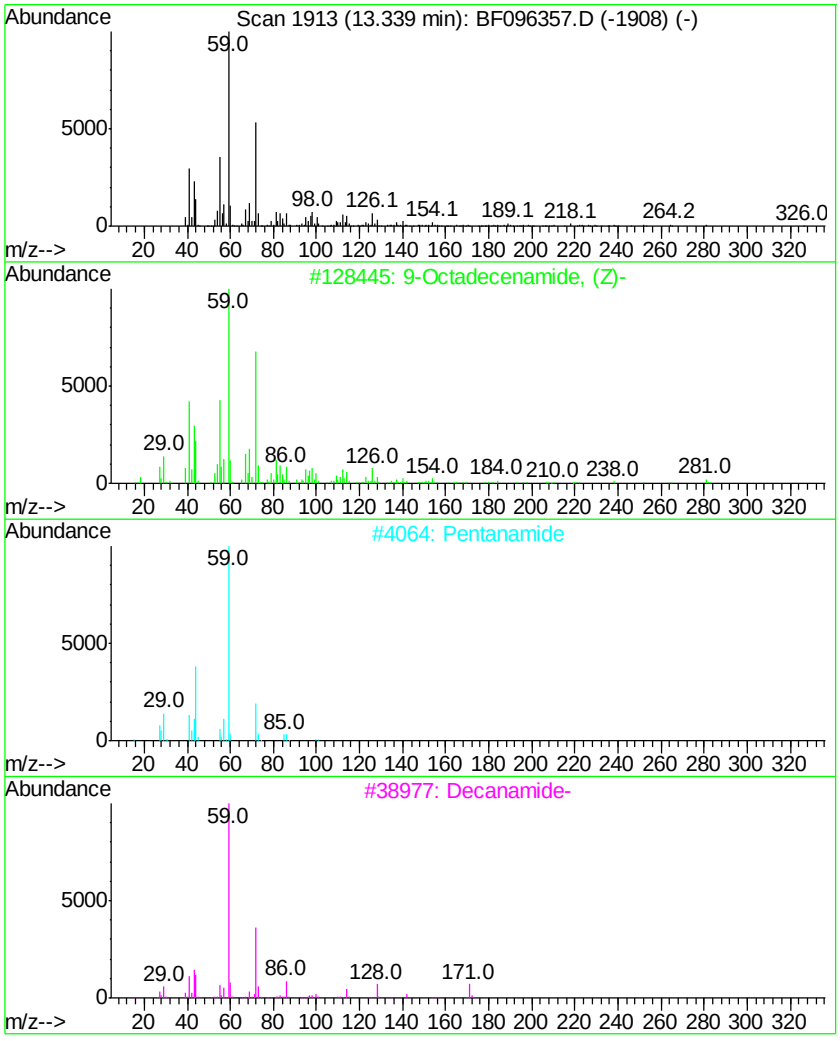
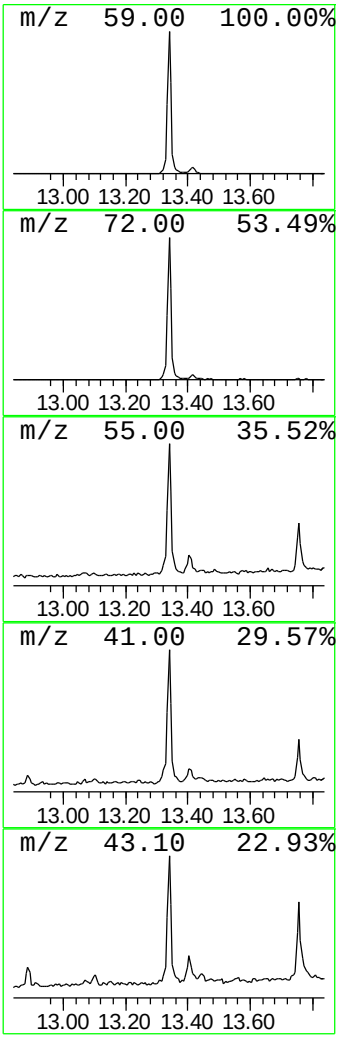
Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	12.33 ng	736660	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Pentanamide	101	C5H11NO	000626-97-1	59
3	Decanamide-	171	C10H21NO	002319-29-1	56
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	2-Pentanol, 3-chloro-2-methyl-	136	C6H13ClO	074685-49-7	47





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Sample : I3930-04
Misc :
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Instrument : BNA_F
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TIC Integration Parameters: LSCINT.P

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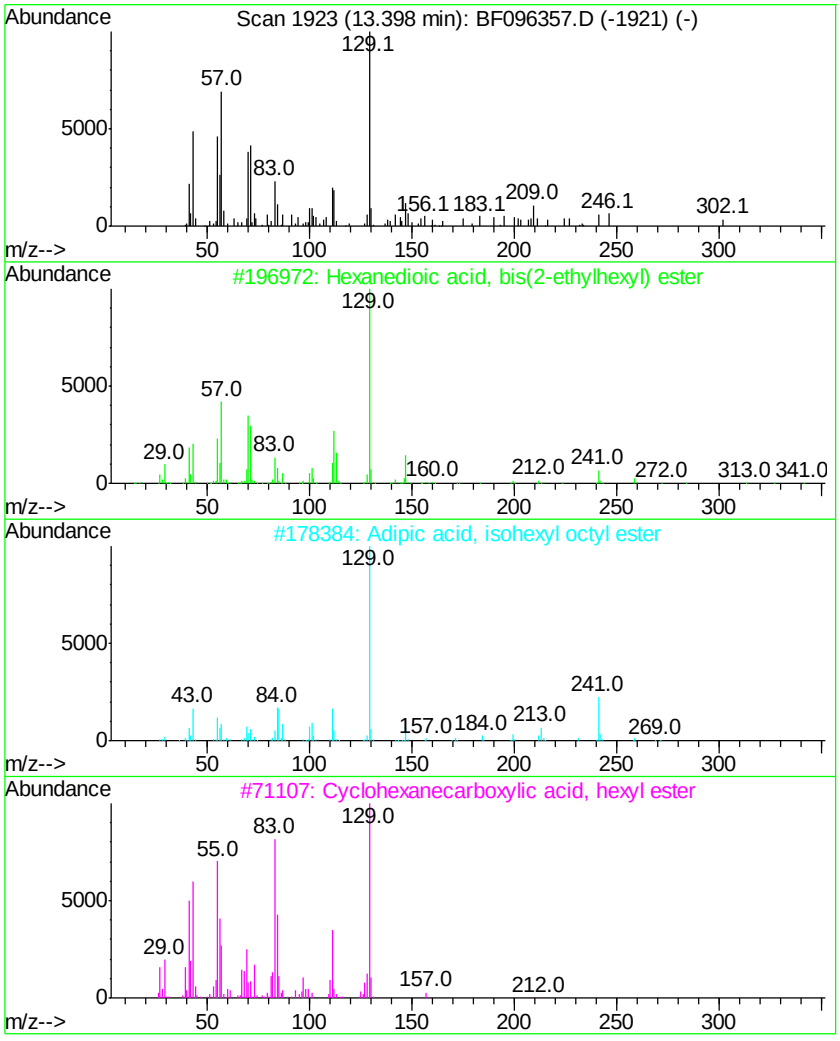
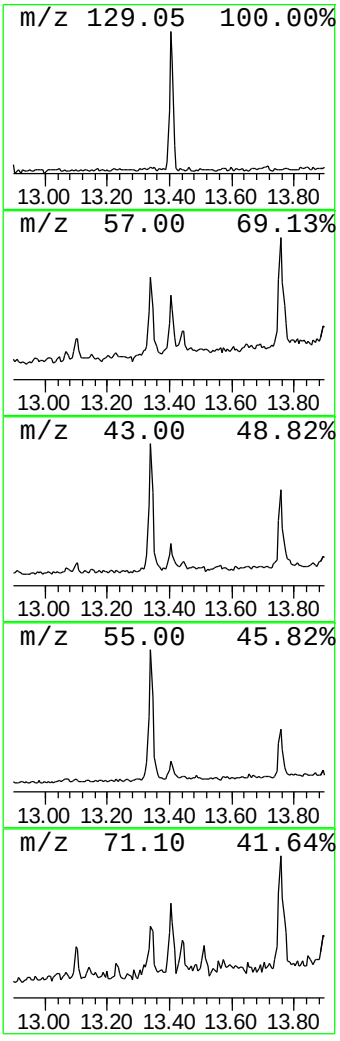
Peak Number 9 Hexanedioic acid, bis(2-eth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.40 ng	143210	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	68
2	Adipic acid, isohexyl octyl ester	342	C20H38O4	1000324-47-0	53
3	Cyclohexanecarboxylic acid, hexy...	212	C13H24O2	027948-10-3	52
4	Adipic acid, cycloheptyl isohexy...	326	C19H34O4	1000324-71-8	50
5	Adipic acid, 3-heptyl octyl ester	356	C21H40O4	1000353-65-3	50





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Data File : BF096357.D
Acq On : 1 Jul 2017 1:00
Operator : SJ/MA
Sample : I3930-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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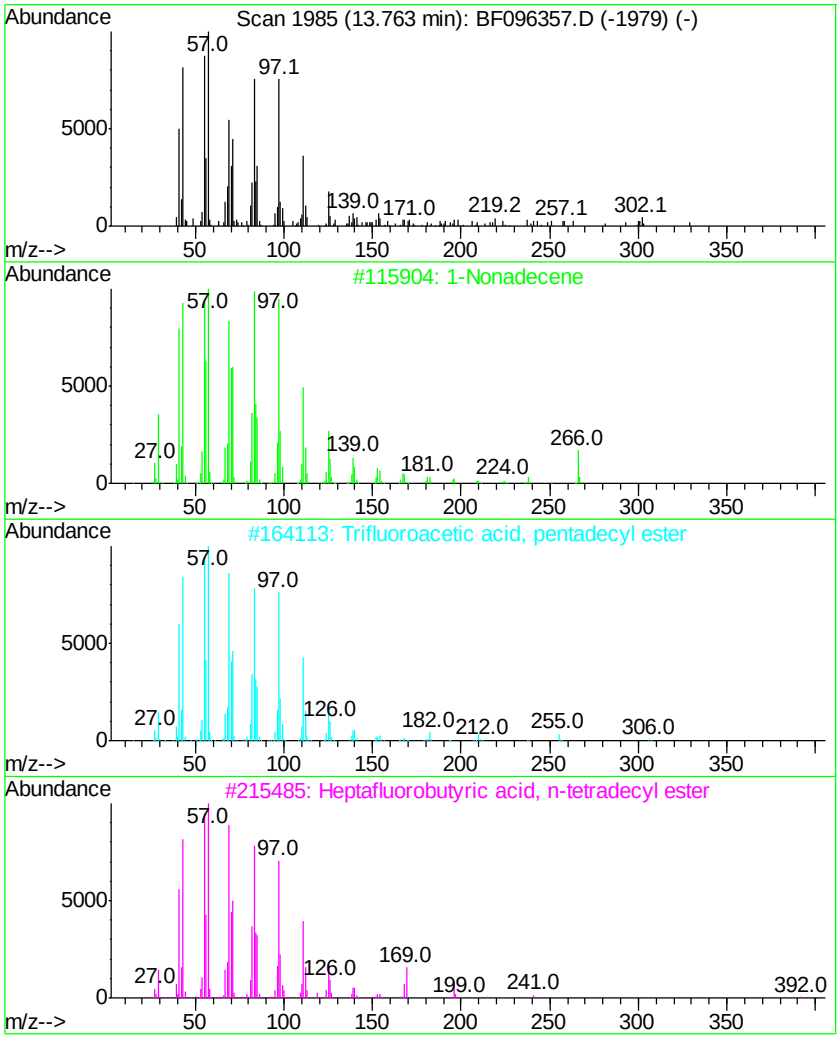
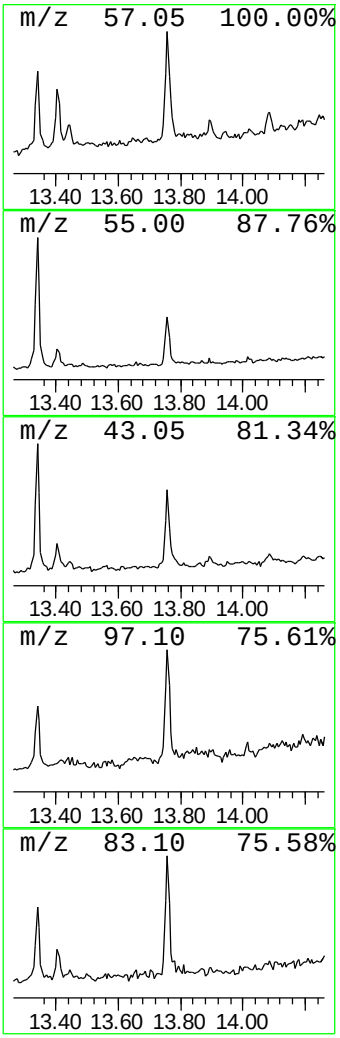
Peak Number 10 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	4.94 ng	295209	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	94
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
4	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





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Data File : BF096357.D
Acq On : 1 Jul 2017 1:00
Operator : SJ/MA
Sample : I3930-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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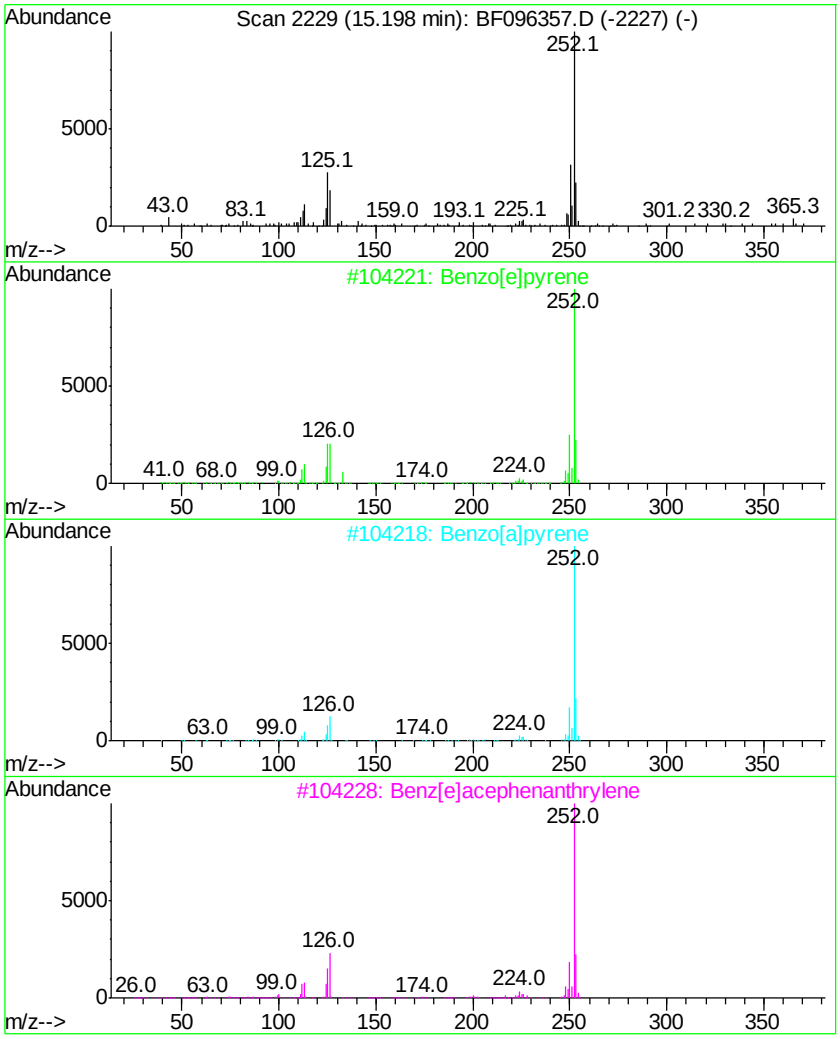
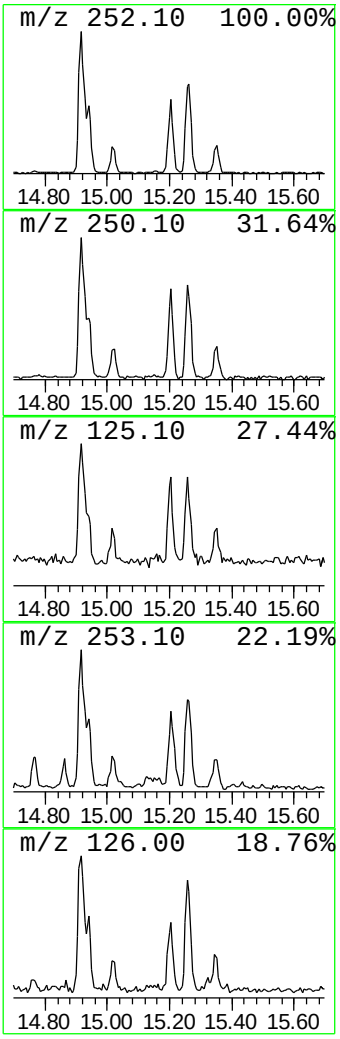
Peak Number 11 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	6.22 ng	159258	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
5	Perylene	252	C20H12	000198-55-0	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096357.D
Acq On : 1 Jul 2017 1:00
Operator : SJ/MA
Sample : I3930-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-6-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	13.7	ng	650837	1	6.76	947689	20.0
unknown6.53	6.53	77.4	ng	3667860	1	6.76	947689	20.0
Tridecane	10.71	3.2	ng	141169	4	11.27	876307	20.0
Pentadecanoic acid	11.81	7.8	ng	339900	4	11.27	876307	20.0
Benzoic acid, 3-a...	11.84	3.0	ng	133327	4	11.27	876307	20.0
Anthracene, 1-met...	11.88	3.3	ng	143492	4	11.27	876307	20.0
9-Octadecenamide,...	13.34	12.3	ng	736660	5	13.90	1194730	20.0
Hexanedioic acid,...	13.40	2.4	ng	143210	5	13.90	1194730	20.0
1-Nonadecene	13.76	4.9	ng	295209	5	13.90	1194730	20.0
Benzo[e]pyrene	15.20	6.2	ng	159258	6	15.32	511728	20.0