LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096624.D
Acq On : 11 Jul 2017 1:56
Operator : SJ/JU
Sample : I4119-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-070717-B

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-BF070117.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	3.016	156	158	168	rBV	65271	135917	4.61%	0.517%
2	4.875	470	474	485	rBV	404033	562031	19.08%	2.139%
3	5.304	541	547	550	rBV	2704552	2848636	96.68%	10.841%
4	5.410	556	565	571	rVB2	23758	47403	1.61%	0.180%
5	6.328	711	721	724	rBV	2706312	2946404	100.00%	11.213%
6	6.457	738	743	746	rBV	2979696	2803245	95.14%	10.668%
7	6.522	751	754	755	rBV	38741	31678	1.08%	0.121%
8	6.687	778	782	785	rBV	949388	809912	27.49%	3.082%
9	6.845	802	809	812	rBV	2339037	2246683	76.25%	8.550%
10	7.245	872	877	880	rBV	1703163	1743130	59.16%	6.634%
11	7.298	880	886	890	rVB2	35958	36436	1.24%	0.139%
12	7.369	890	898	901	rBV	111312	153608	5.21%	0.585%
13	7.875	980	984	988	rBV	58235	52057	1.77%	0.198%
14	7.969	995	1000	1003	rBV	1010107	876626	29.75%	3.336%
15	9.045	1178	1183	1186	rBV	2863089	2645277	89.78%	10.067%
16	9.439	1245	1250	1253	rBV	715543	620477	21.06%	2.361%
17	9.716	1292	1297	1301	rBV2	877401	775148	26.31%	2.950%
18	9.928	1324	1333	1336	rBV3	19239	31306	1.06%	0.119%
19	10.504	1426	1431	1434	rBV	1231082	1188047	40.32%	4.521%
20	10.633	1450	1453	1463	rVB	58105	73003	2.48%	0.278%
21	11.080	1526	1529	1533	rBV2	53280	49900	1.69%	0.190%
22	11.192	1545	1548	1551	rBV	686848	613749	20.83%	2.336%
23	11.216	1551	1552	1555	rVB	143794	86509	2.94%	0.329%
24	11.269	1555	1561	1564	rVB	58664	51503	1.75%	0.196%
25	11.433	1585	1589	1595	rBV2	185049	170070	5.77%	0.647%
26	11.604	1614	1618	1623	rVB5	25284	31842	1.08%	0.121%
27	11.698	1631	1634	1636	rBV	53775	52933	1.80%	0.201%
28	11.722	1636	1638	1643	rVB2	71347	88739	3.01%	0.338%
29	11.804	1649	1652	1654	rBV	74782	72804	2.47%	0.277%
30	11.827	1654	1656	1659	rVB	48225	37939	1.29%	0.144%
31	12.010	1685	1687	1694	rVB5	34578	42229	1.43%	0.161%
32	12.251	1724	1728	1731	rBV2	286909	289253	9.82%	1.101%
33	12.404	1750	1754	1757	rVB	195888	181797	6.17%	0.692%
34	12.627	1787	1792	1795	rBV	257919	256129	8.69%	0.975%

LSC Area Percent Report

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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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.780	1814	1818	1821	rBV	1846473	1709306	58.01%	6.505%
36	12.851	1827	1830	1833	rBV3	36384	41259	1.40%	0.157%
37	12.957	1846	1848	1852	rVB	45282	41862	1.42%	0.159%
38	13.063	1862	1866	1869	rBV	57256	63836	2.17%	0.243%
39	13.151	1879	1881	1884	rBV	46210	40719	1.38%	0.155%
40	13.186	1884	1887	1890	rBV2	45806	46958	1.59%	0.179%
41	13.233	1892	1895	1898	rVB5	30143	43277	1.47%	0.165%
42	13.568	1949	1952	1956	rBV2	33736	42949	1.46%	0.163%
43	13.680	1968	1971	1979	rBV3	116677	150896	5.12%	0.574%
44	13.821	1991	1995	1998	rBV	678190	743396	25.23%	2.829%
45	13.845	1998	1999	2002	rVB	99561	72323	2.45%	0.275%
46	14.680	2138	2141	2145	rVB	85491	91661	3.11%	0.349%
47	15.163	2221	2223	2226	rBV	64756	52667	1.79%	0.200%
48	15.227	2229	2234	2237	rBV	416103	483489	16.41%	1.840%

Sum of corrected areas: 26277018

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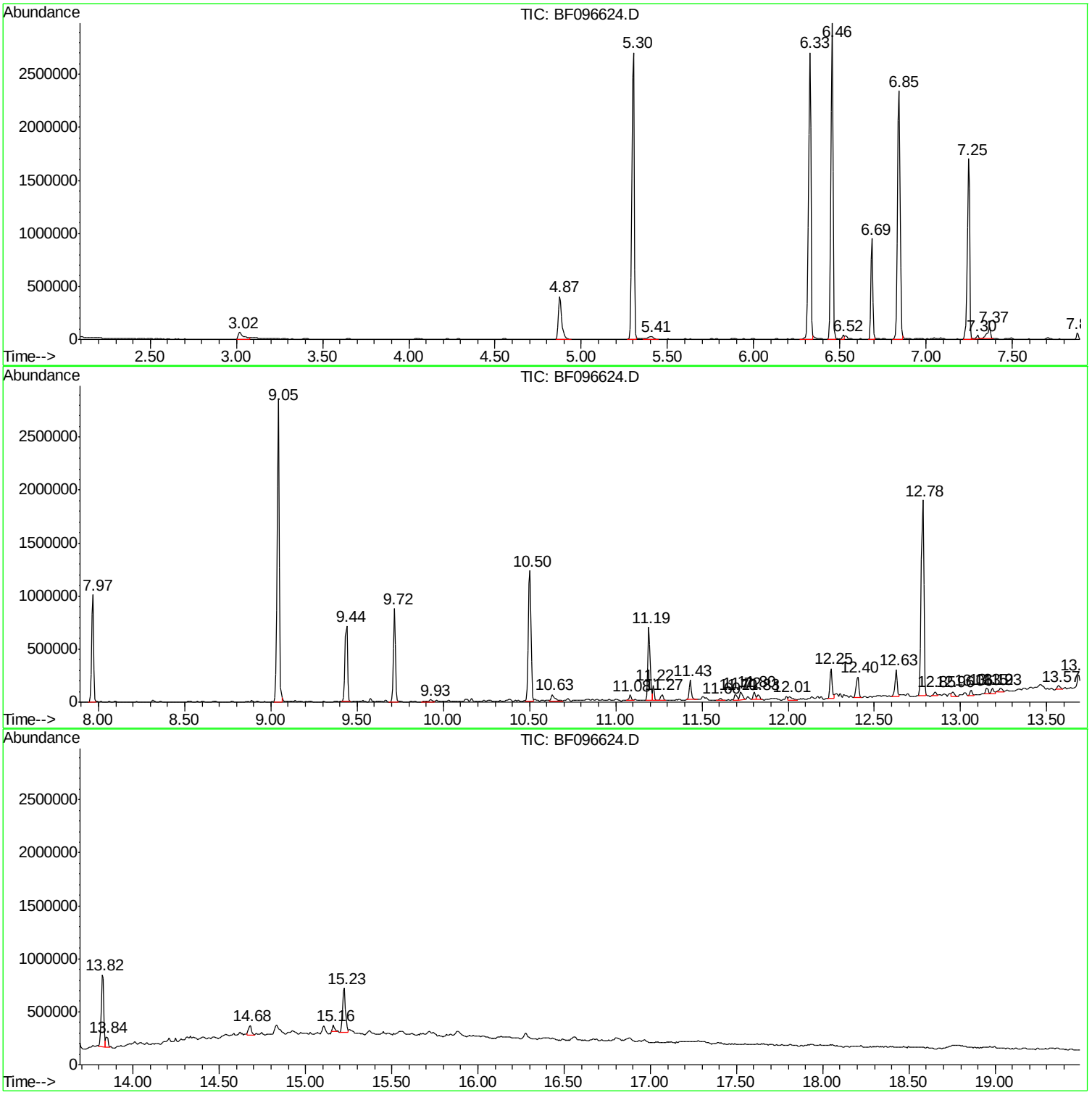
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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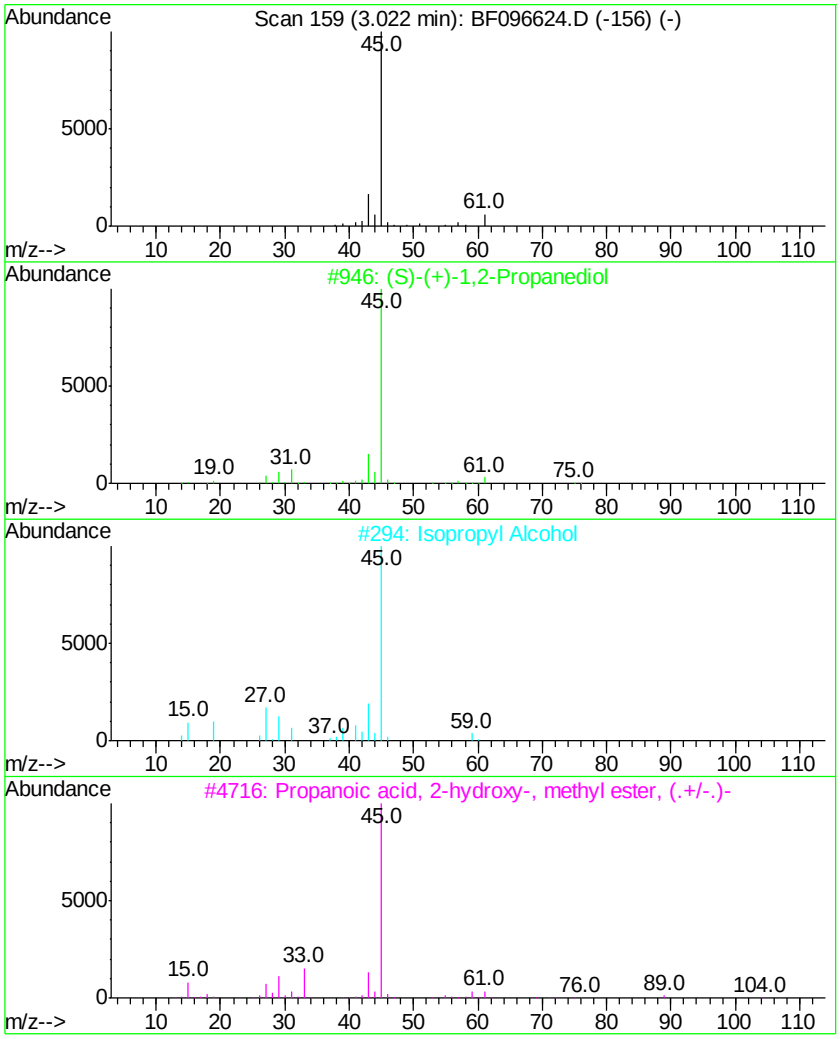
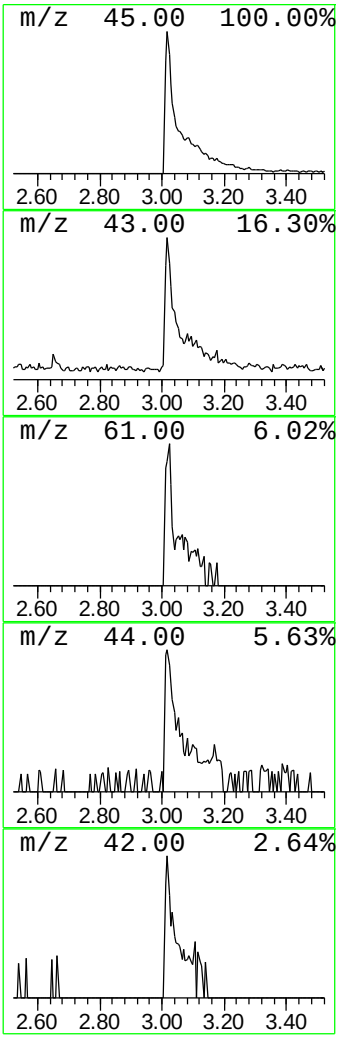
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	3.36 ng	135917	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
4	Methyltartronic acid	134	C4H6O5	000595-98-2	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





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Instrument : BNA_F
ClientSampleId : EO-03-070717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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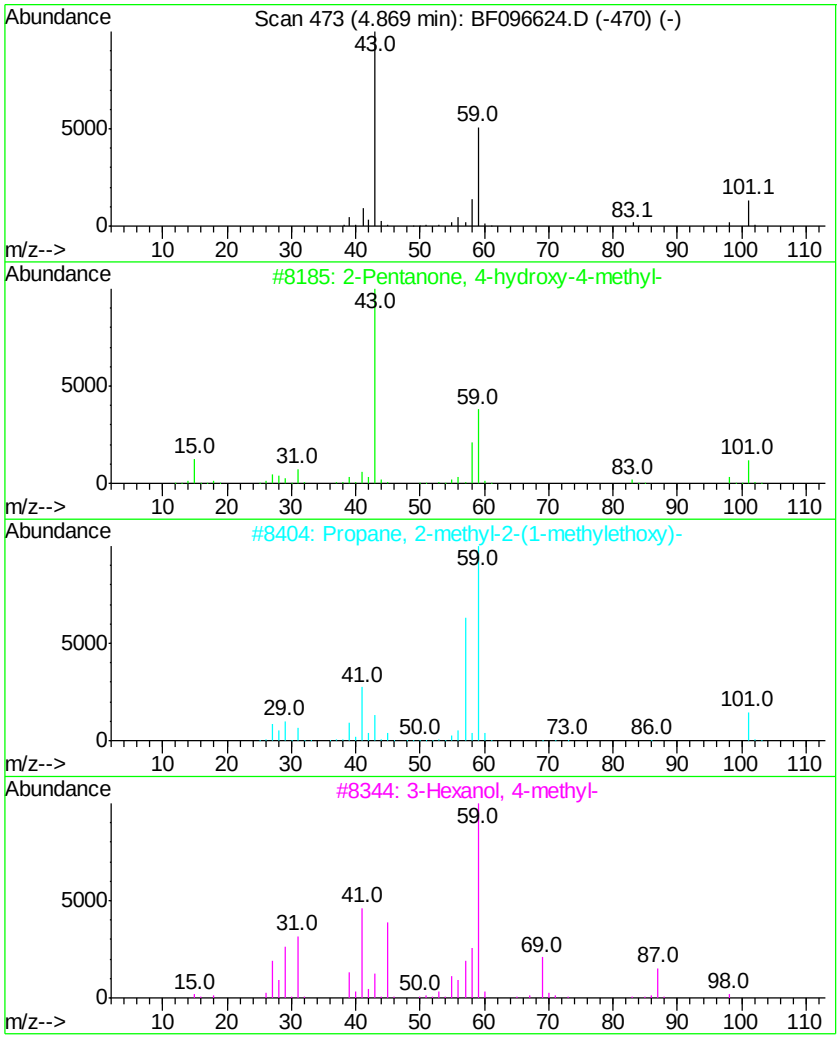
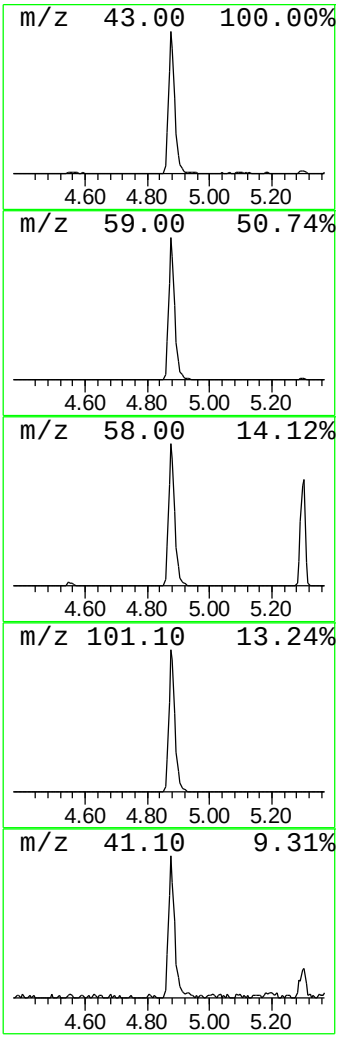
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	13.88 ng	562031	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33





Library Search Compound Report

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ClientSampleId : EO-03-070717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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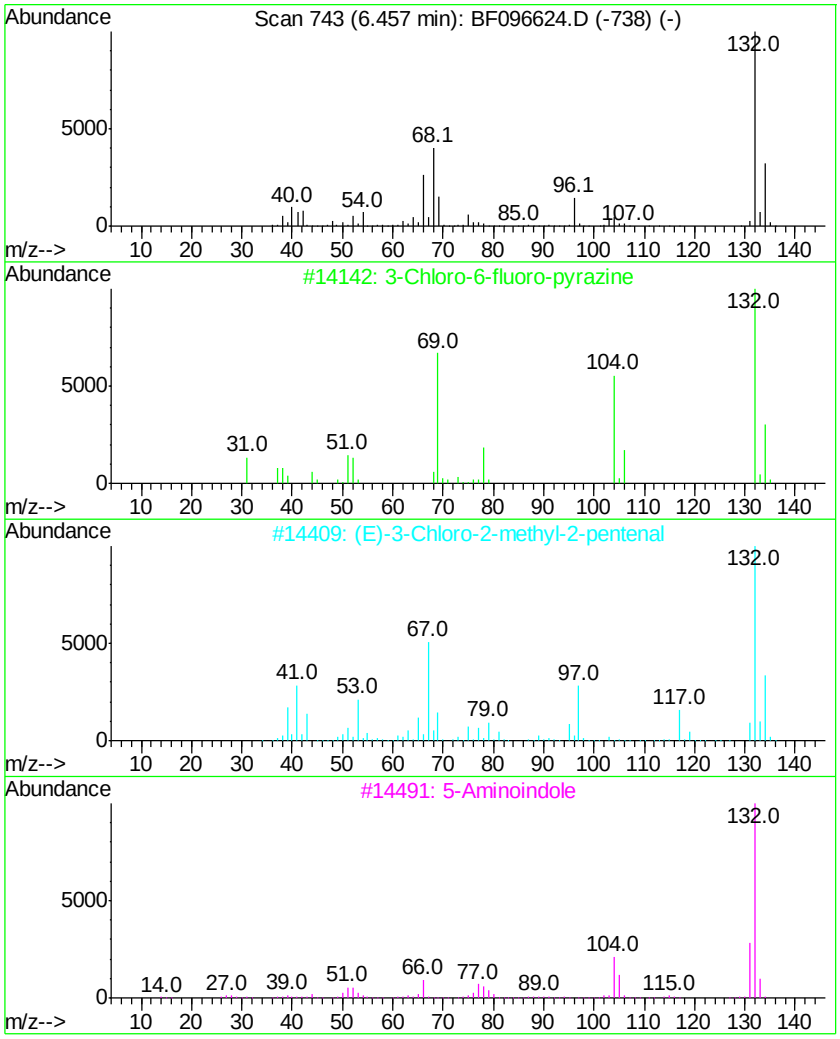
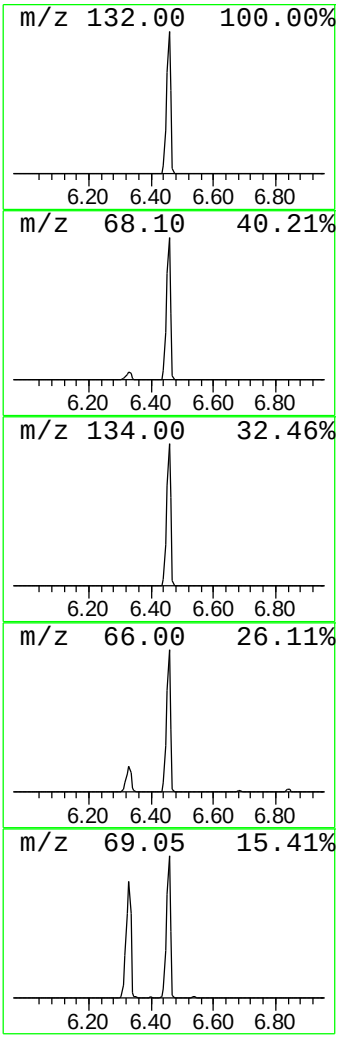
Peak Number 3 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	69.22 ng	2803250	1,4-Dichlorobenzene-d4	6.69

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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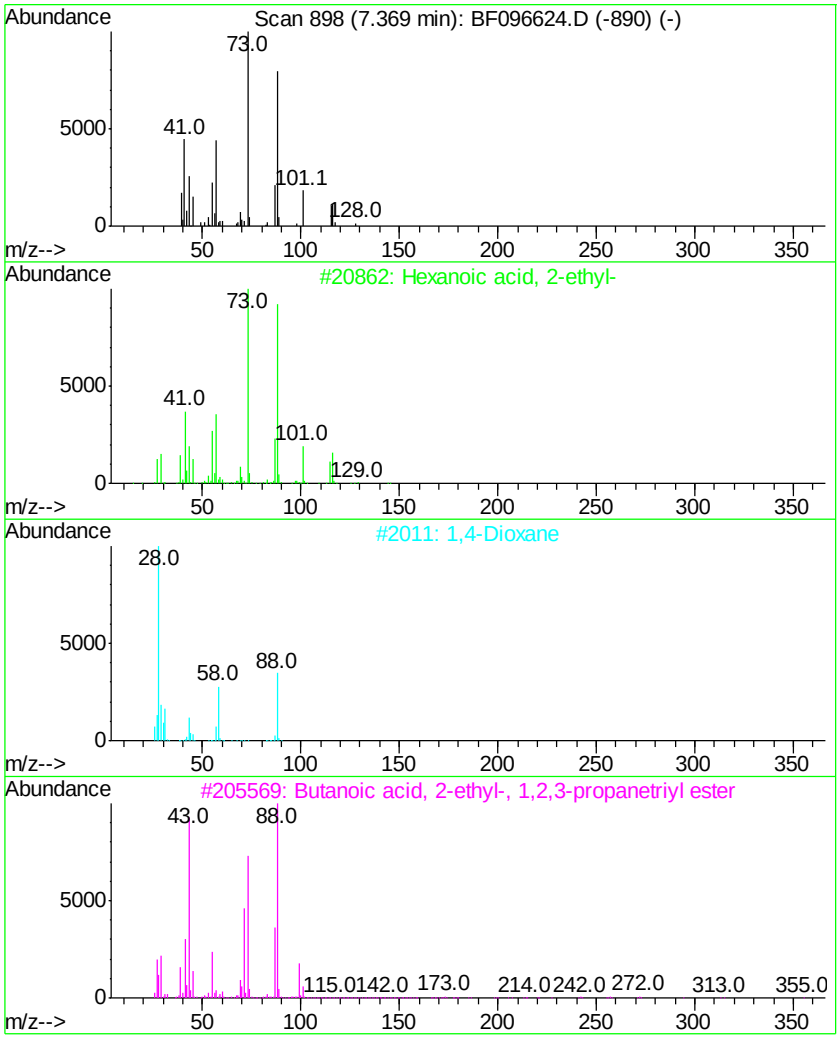
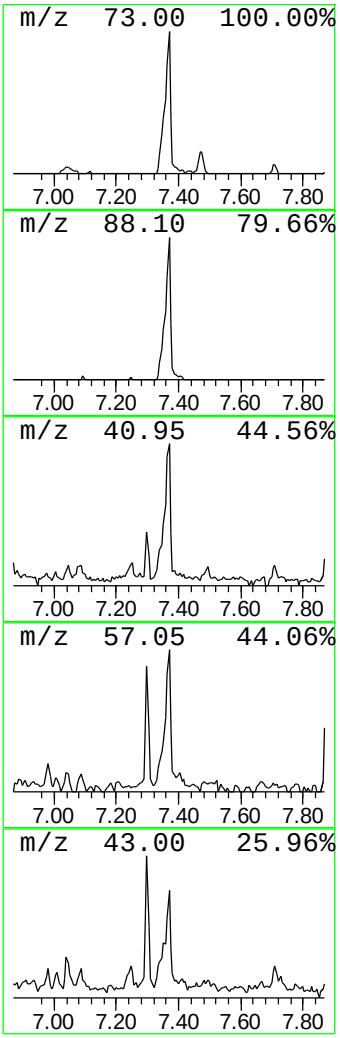
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	3.50 ng	153608	Naphthalene-d8	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	1,4-Dioxane	88	C4H8O2	000123-91-1	47
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
4	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	36
5	Methyl 4-O-acetyl-2,3-di-O-methy...	248	C11H20O6	072945-56-3	33





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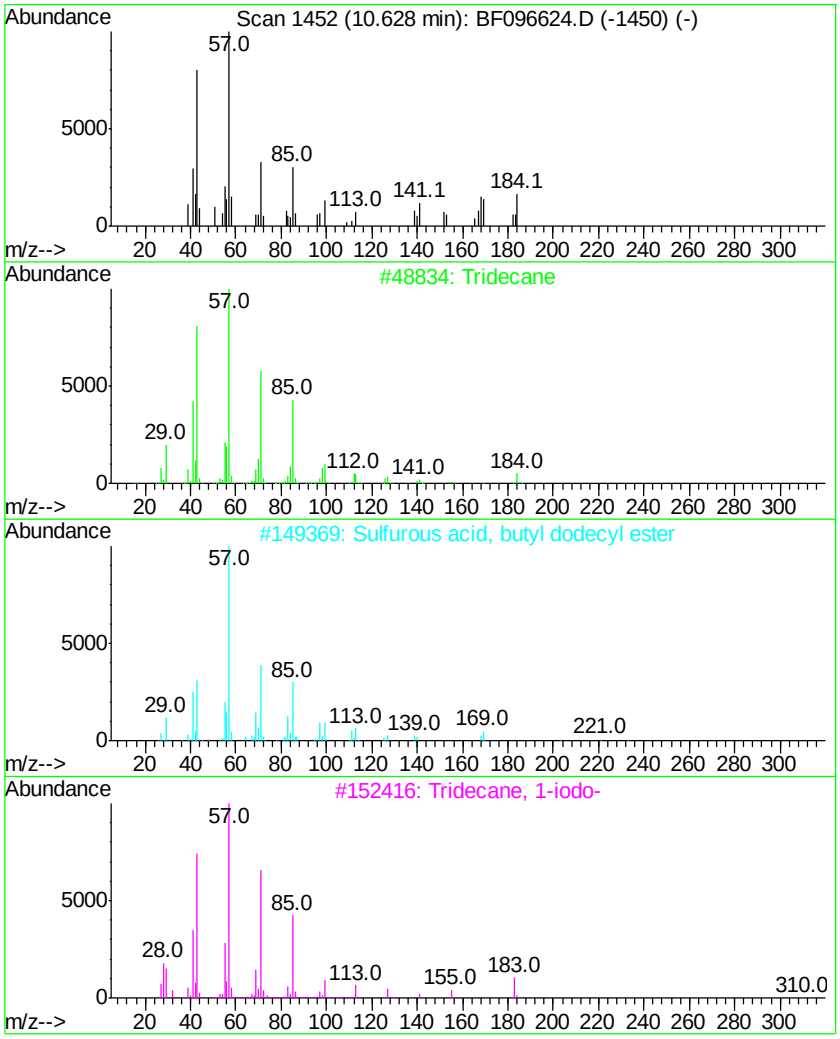
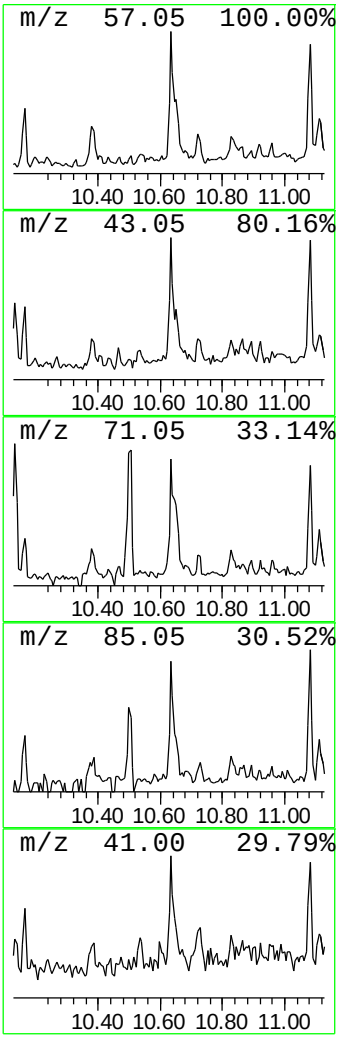
Peak Number 6 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.38 ng	73003	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	86
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
4	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	64
5	Tetratetracontane	619	C44H90	007098-22-8	59





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TIC Library : C:\DATABASE\NIST11.L
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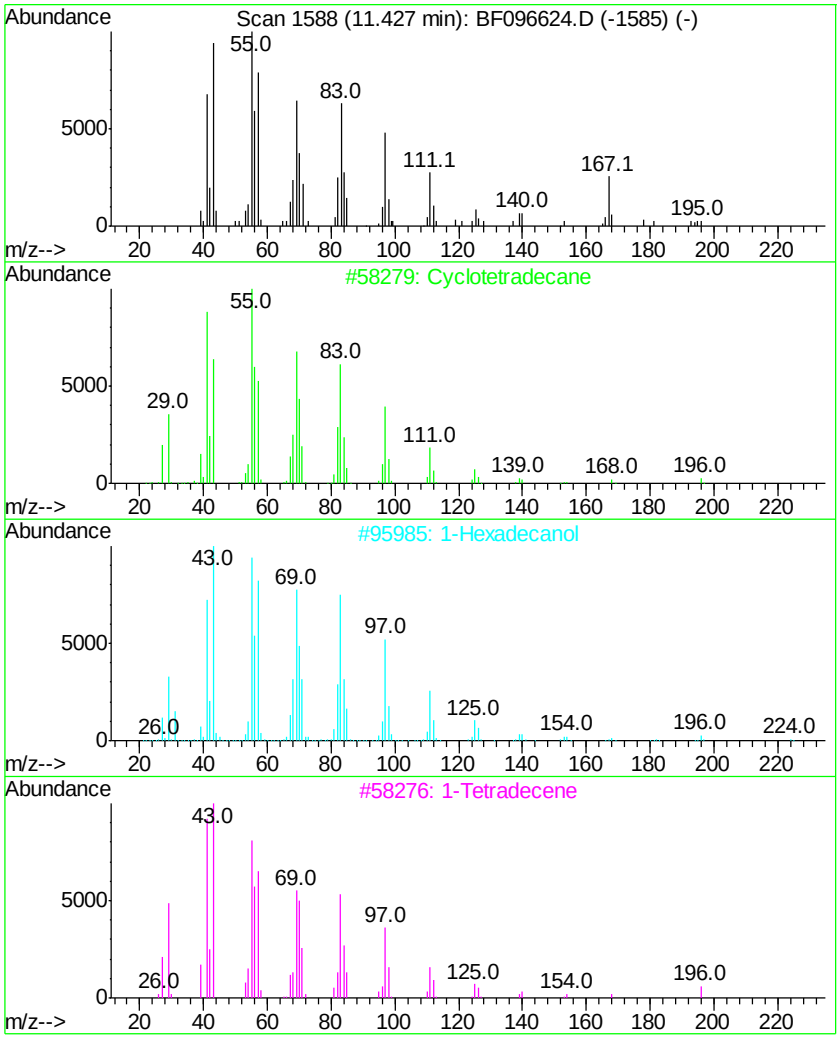
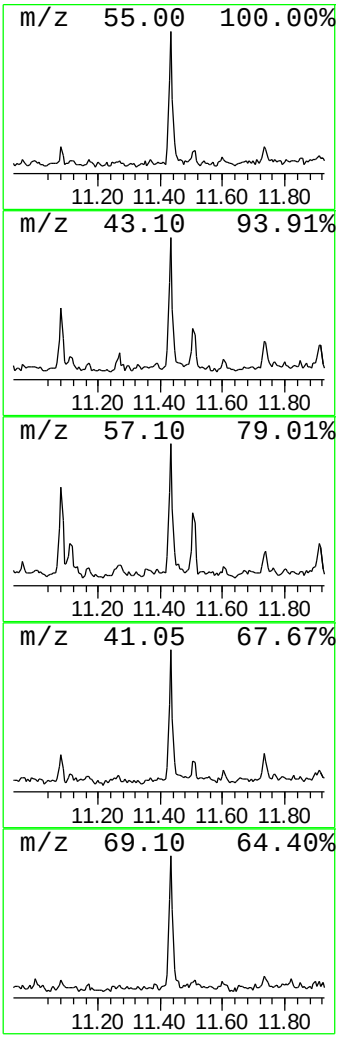
Peak Number 7 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	5.54 ng	170070	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	97
2	1-Hexadecanol	242	C16H34O	036653-82-4	95
3	1-Tetradecene	196	C14H28	001120-36-1	95
4	Cetene	224	C16H32	000629-73-2	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91





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

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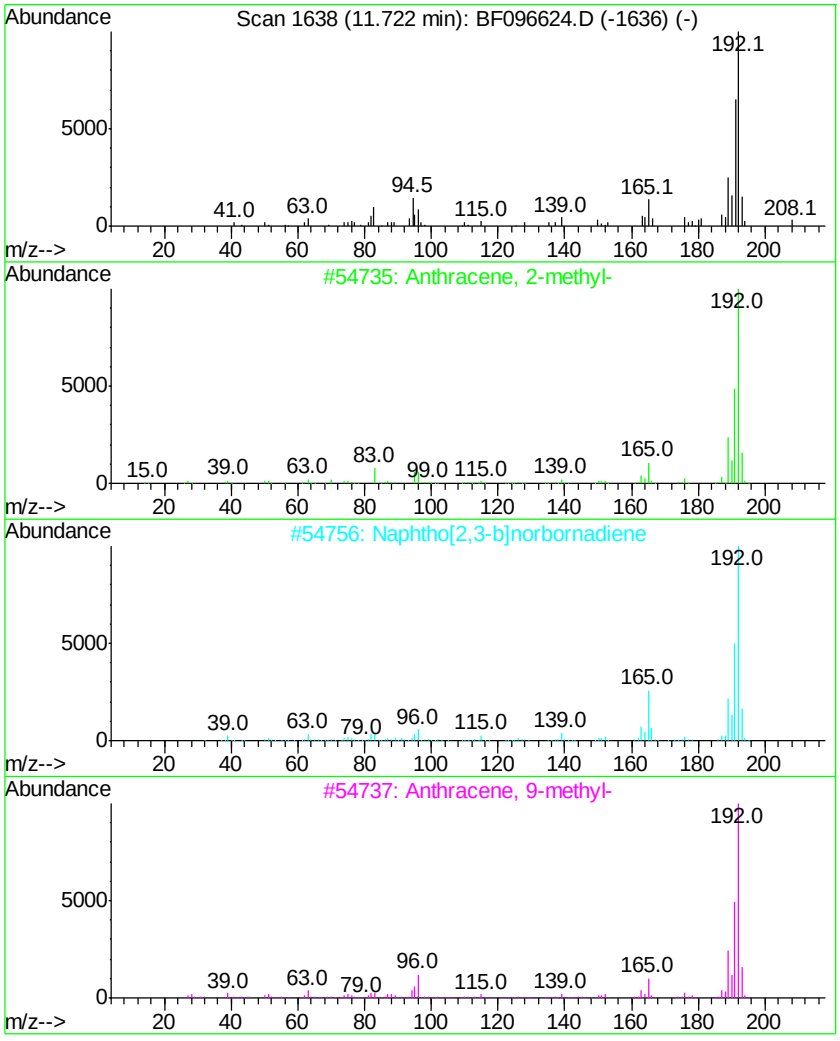
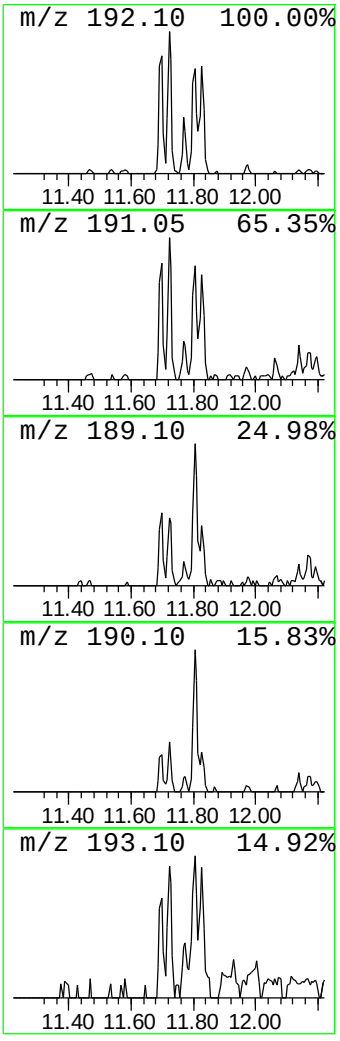
Peak Number 8 Anthracene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	2.89 ng	88739	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	93
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90





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Instrument : BNA_F
ClientSampleId : EO-03-070717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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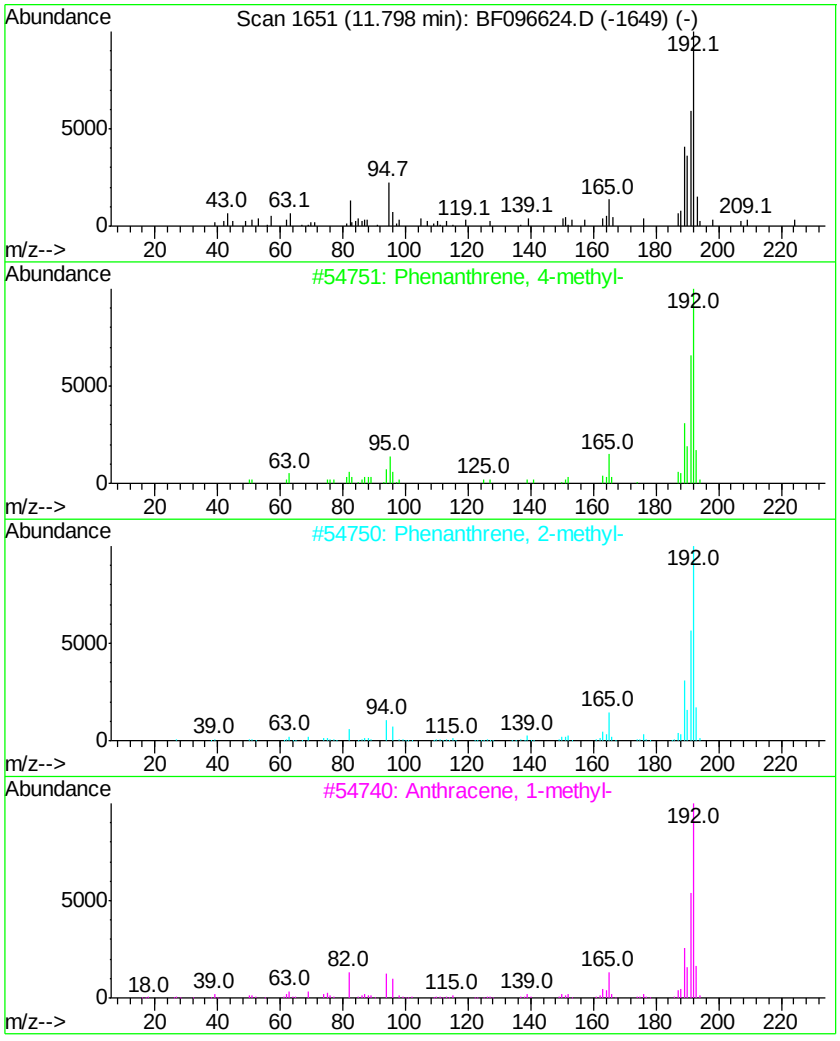
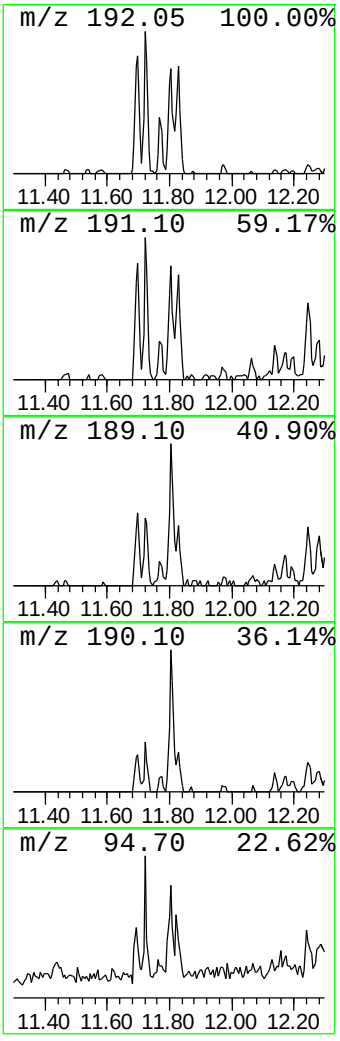
Peak Number 9 Phenanthrene, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.37 ng	72804	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	60
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	53





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Data File : BF096624.D
Acq On : 11 Jul 2017 1:56
Operator : SJ/JU
Sample : I4119-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-070717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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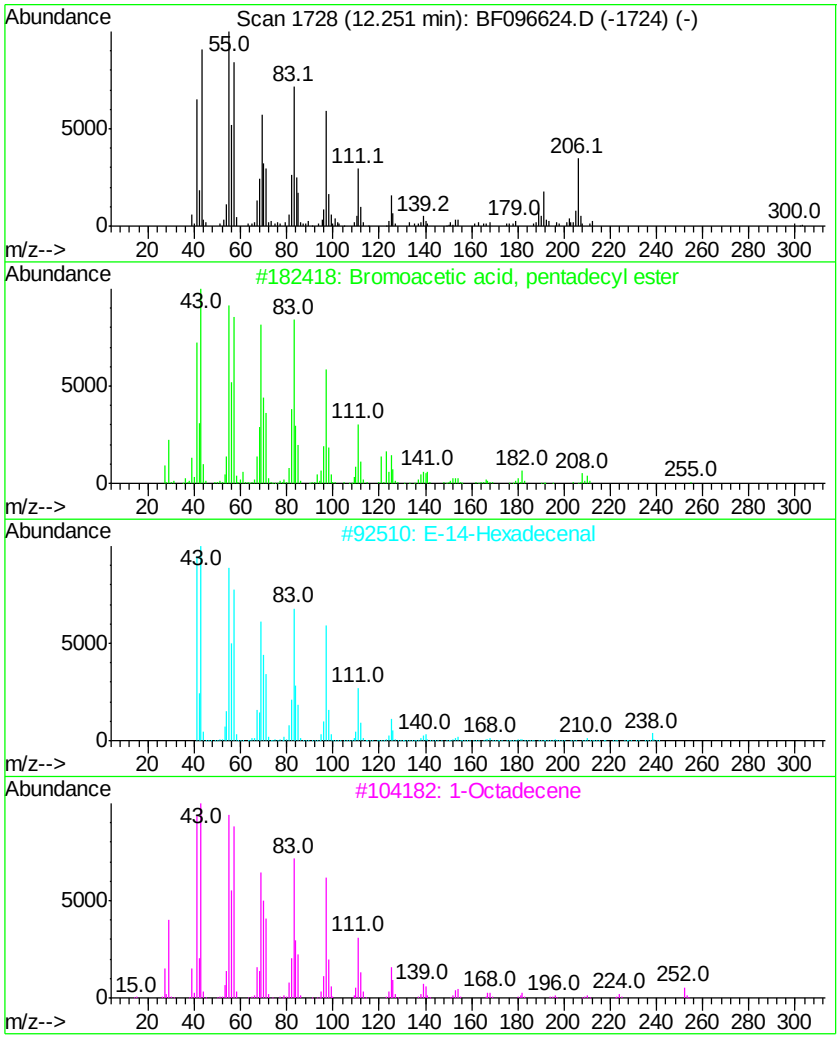
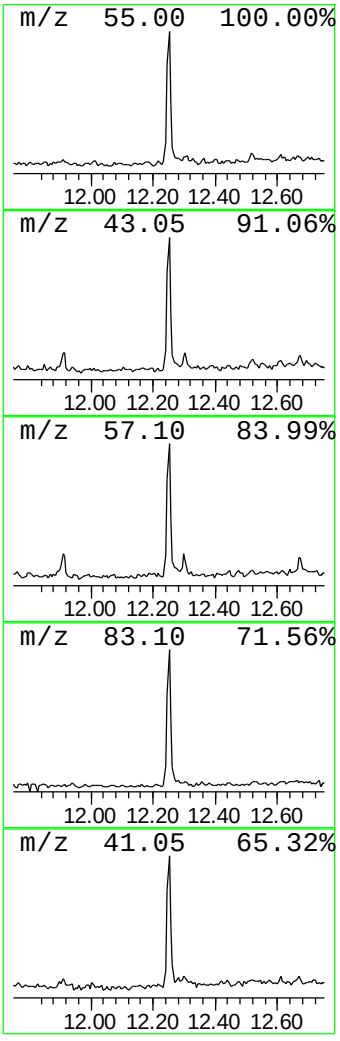
Peak Number 10 Bromoacetic acid, pentadecy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	9.43 ng	289253	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	87
3	1-Octadecene	252	C18H36	000112-88-9	87
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	87
5	11-Tricosene	322	C23H46	052078-56-5	83





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Data File : BF096624.D
Acq On : 11 Jul 2017 1:56
Operator : SJ/JU
Sample : I4119-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-070717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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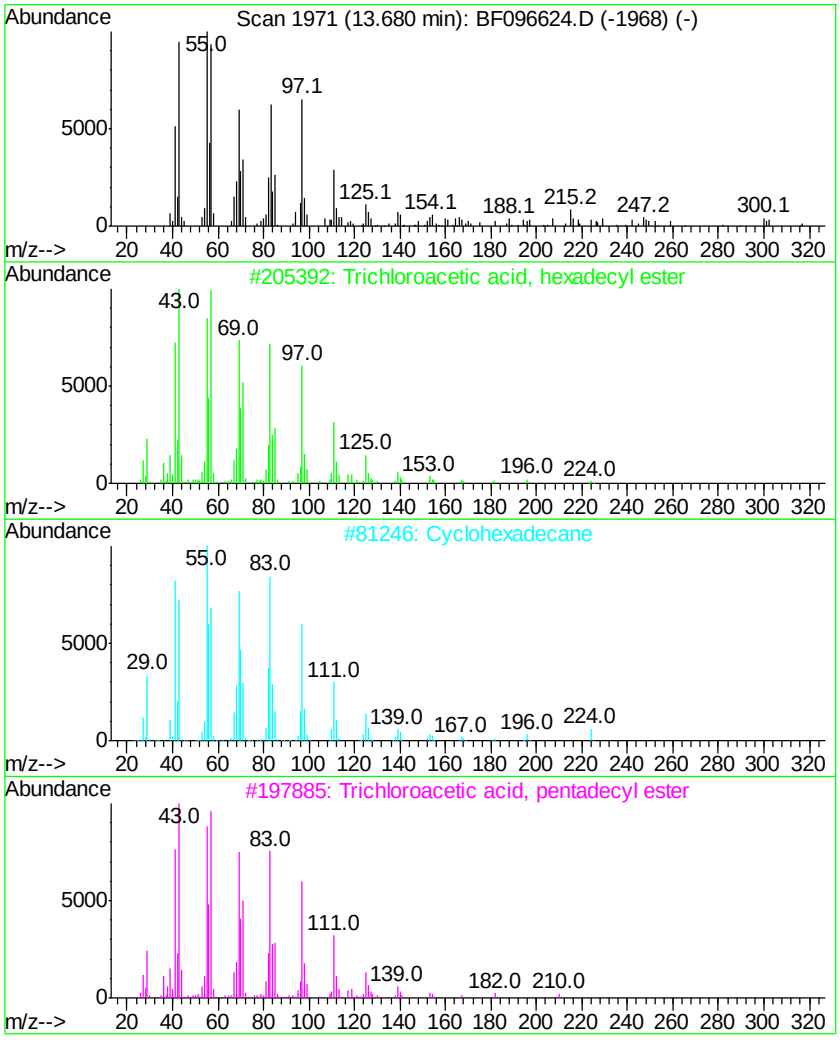
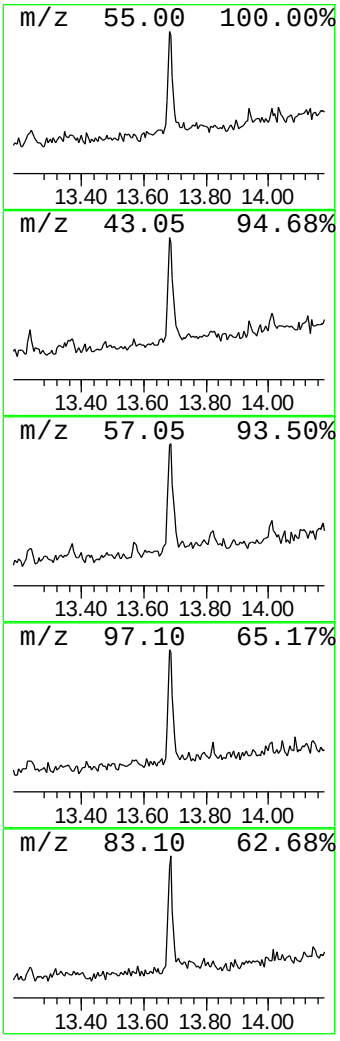
Peak Number 11 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	4.06 ng	150896	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	Cyclohexadecane	224	C16H32	000295-65-8	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
5	1,2-Octadecanediol	286	C18H38O2	020294-76-2	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096624.D
Acq On : 11 Jul 2017 1:56
Operator : SJ/JU
Sample : I4119-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-070717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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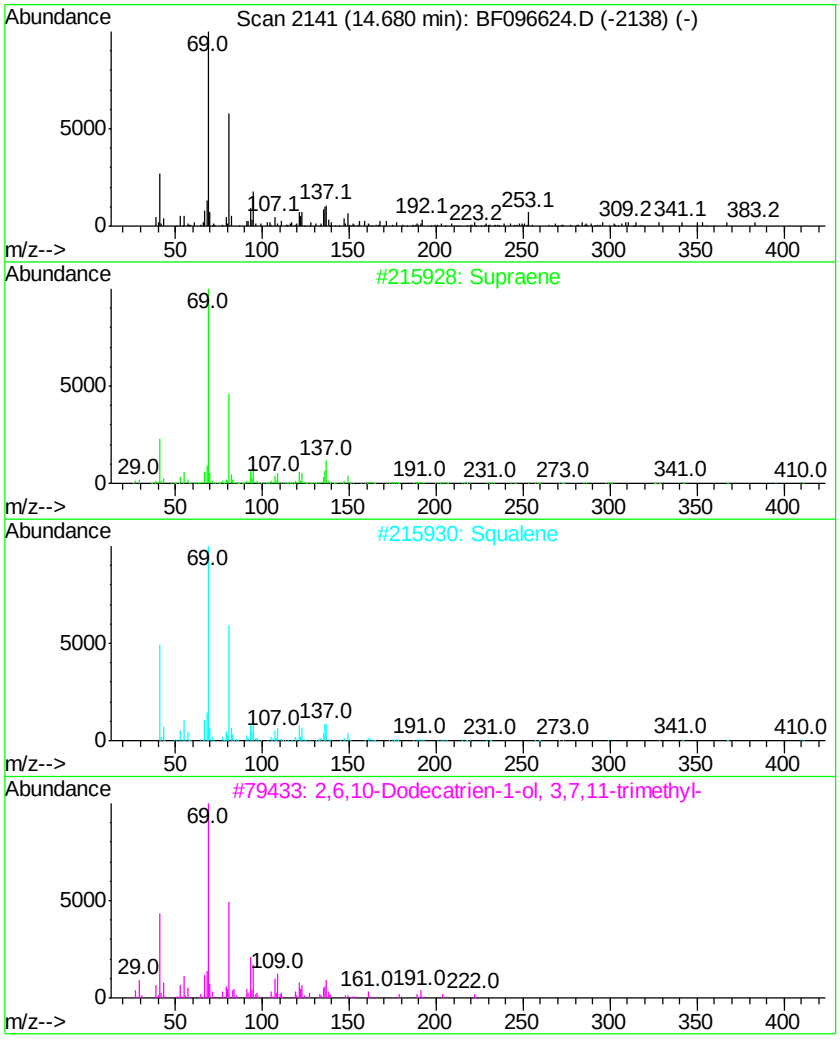
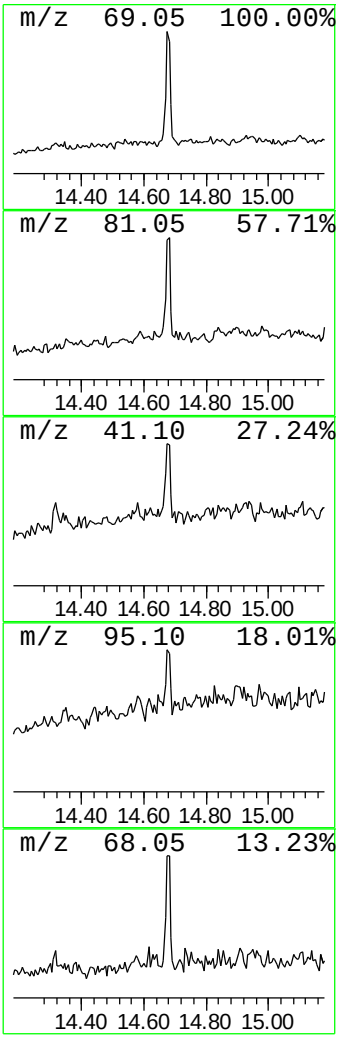
Peak Number 12 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	3.79 ng	91661	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	Squalene	410	C30H50	000111-02-4	80
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
4	2,6,10-Dodecatrienoic acid, 3,7,...	264	C17H28O2	019954-66-6	72
5	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096624.D
Acq On : 11 Jul 2017 1:56
Operator : SJ/JU
Sample : I4119-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-070717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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
(S)-(+)-1,2-Propa...	3.02	3.4	ng	135917	1	6.69	809912	20.0
2-Pentanone, 4-hy...	4.87	13.9	ng	562031	1	6.69	809912	20.0
unknown6.46	6.46	69.2	ng	2803250	1	6.69	809912	20.0
Hexanoic acid, 2-...	7.37	3.5	ng	153608	2	7.97	876626	20.0
Tridecane	10.63	2.4	ng	73003	4	11.19	613749	20.0
Cyclotetradecane	11.43	5.5	ng	170070	4	11.19	613749	20.0
Anthracene, 2-met...	11.72	2.9	ng	88739	4	11.19	613749	20.0
Phenanthrene, 4-m...	11.80	2.4	ng	72804	4	11.19	613749	20.0
Bromoacetic acid,...	12.25	9.4	ng	289253	4	11.19	613749	20.0
Trichloroacetic a...	13.68	4.1	ng	150896	5	13.83	743396	20.0
Supraene	14.68	3.8	ng	91661	6	15.23	483489	20.0