LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096798.D
Acq On : 15 Jul 2017 3:38
Operator : SJ/JU
Sample : I4187-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

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-BF071317.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	2.904	153	156	164	rBV	29859	61695	2.56%	0.282%
2	4.804	475	479	490	rBV	198528	278195	11.54%	1.270%
3	5.240	548	553	556	rBV	2408758	2411643	100.00%	11.009%
4	6.281	724	730	738	rVB	2011948	2181296	90.45%	9.958%
5	6.398	746	750	753	rBV	2333247	2141424	88.80%	9.776%
6	6.628	785	789	792	rBV	684251	608987	25.25%	2.780%
7	6.781	811	815	819	rBV	1758753	1659919	68.83%	7.578%
8	7.186	879	884	887	rBV	1298372	1336303	55.41%	6.100%
9	7.310	901	905	910	rVB	39522	40848	1.69%	0.186%
10	7.822	989	992	997	rBV	37941	33583	1.39%	0.153%
11	7.910	1003	1007	1010	rBV	962385	882320	36.59%	4.028%
12	8.598	1117	1124	1126	rBV	76764	70829	2.94%	0.323%
13	8.986	1185	1190	1193	rBV	2278582	2043791	84.75%	9.330%
14	9.380	1253	1257	1260	rBV	437134	369960	15.34%	1.689%
15	9.657	1299	1304	1307	rBV	752029	680612	28.22%	3.107%
16	10.104	1377	1380	1383	rVB	41191	30685	1.27%	0.140%
17	10.439	1433	1437	1441	rBV	1055316	933330	38.70%	4.261%
18	10.574	1457	1460	1468	rBV	48274	55065	2.28%	0.251%
19	11.022	1532	1536	1539	rBV	42434	38491	1.60%	0.176%
20	11.133	1551	1555	1557	rBV	650975	597095	24.76%	2.726%
21	11.151	1557	1558	1562	rVB	53407	37531	1.56%	0.171%
22	11.204	1565	1567	1571	rVB2	31377	27234	1.13%	0.124%
23	11.374	1589	1596	1602	rBV4	49869	53313	2.21%	0.243%
24	11.680	1645	1648	1650	rBV	158660	122935	5.10%	0.561%
25	11.704	1650	1652	1655	rVB	59531	48734	2.02%	0.222%
26	11.921	1686	1689	1692	rBV3	22712	26706	1.11%	0.122%
27	12.339	1756	1760	1763	rBV	164540	137589	5.71%	0.628%
28	12.398	1766	1770	1774	rBV3	19578	28872	1.20%	0.132%
29	12.563	1793	1798	1802	rBV	132058	136292	5.65%	0.622%
30	12.716	1820	1824	1828	rVB	1515992	1437850	59.62%	6.564%
31	12.939	1859	1862	1864	rBV	32723	29329	1.22%	0.134%
32	13.086	1884	1887	1891	rBV5	38499	46872	1.94%	0.214%
33	13.192	1903	1905	1910	rVB	56426	50056	2.08%	0.229%
34	13.510	1956	1959	1962	rVB3	29062	32252	1.34%	0.147%

LSC Area Percent Report

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Sample : I4187-08
Misc :
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Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.621	1975	1978	1984	rVB	228609	235305	9.76%	1.074%
36	13.757	1996	2001	2004	rBV	707136	756165	31.35%	3.452%
37	13.780	2004	2005	2009	rVB	68329	56046	2.32%	0.256%
38	13.951	2031	2034	2036	rBV2	24366	25959	1.08%	0.119%
39	14.257	2083	2086	2097	rVB	187537	223430	9.26%	1.020%
40	14.615	2145	2147	2151	rVB	47755	43551	1.81%	0.199%
41	14.674	2154	2157	2160	rBV	98788	92415	3.83%	0.422%
42	14.757	2168	2171	2178	rVB	79565	142382	5.90%	0.650%
43	14.857	2184	2188	2189	rBV	151352	174540	7.24%	0.797%
44	15.027	2215	2217	2222	rVB	42608	39612	1.64%	0.181%
45	15.080	2224	2226	2231	rVB	55433	61811	2.56%	0.282%
46	15.139	2232	2236	2243	rBV	365383	456141	18.91%	2.082%
47	15.368	2272	2275	2280	rVB	53960	71985	2.98%	0.329%
48	15.580	2307	2311	2315	rBV	142104	202806	8.41%	0.926%
49	15.621	2315	2318	2323	rVB3	71071	105043	4.36%	0.480%
50	16.280	2425	2430	2439	rVB3	88001	164204	6.81%	0.750%
51	16.551	2470	2476	2481	rBV3	59104	139415	5.78%	0.636%
52	16.974	2539	2548	2554	rBV8	78732	242974	10.08%	1.109%

Sum of corrected areas: 21905420

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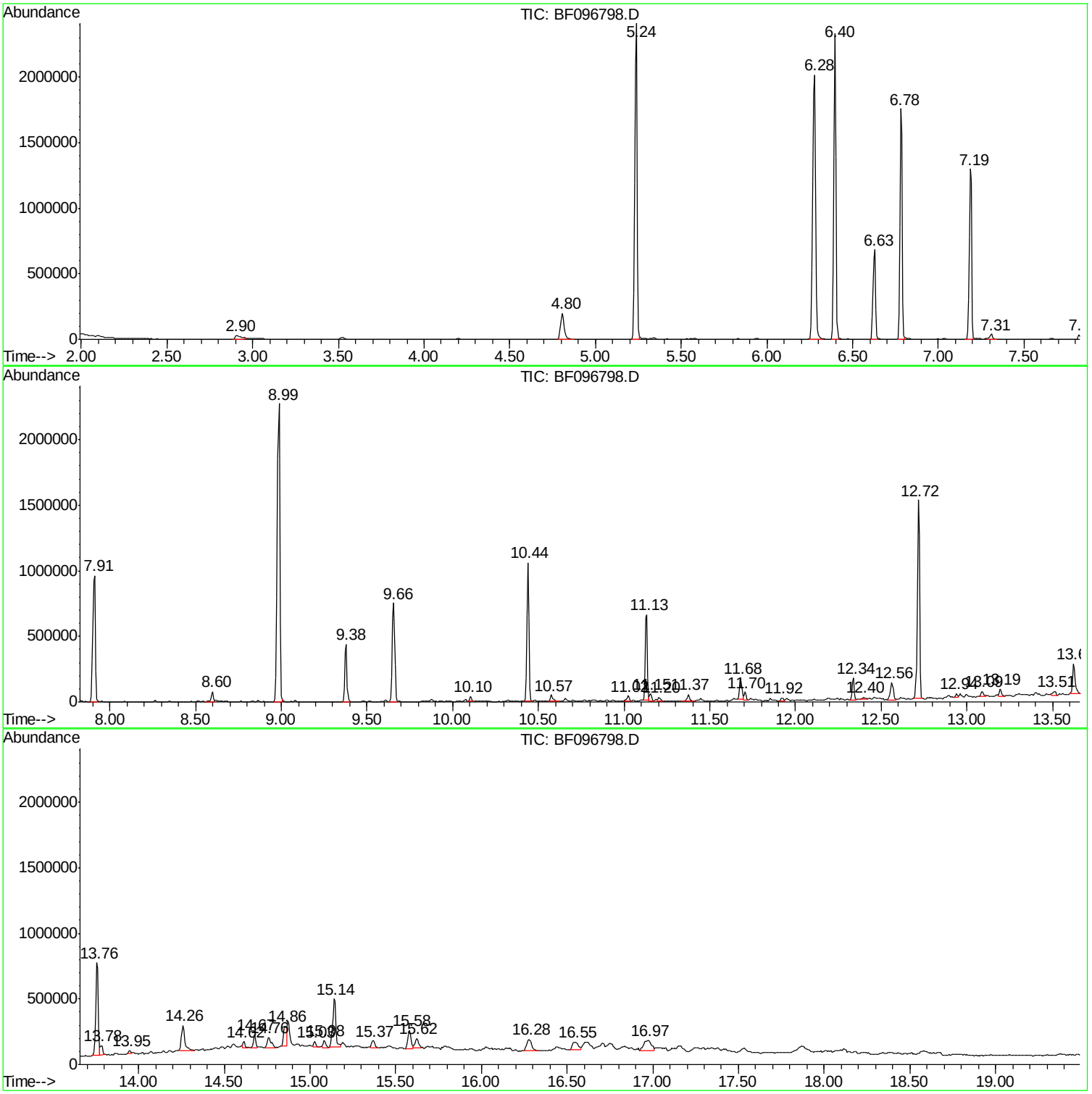
Instrument :
BNA_F
ClientSampleId :
CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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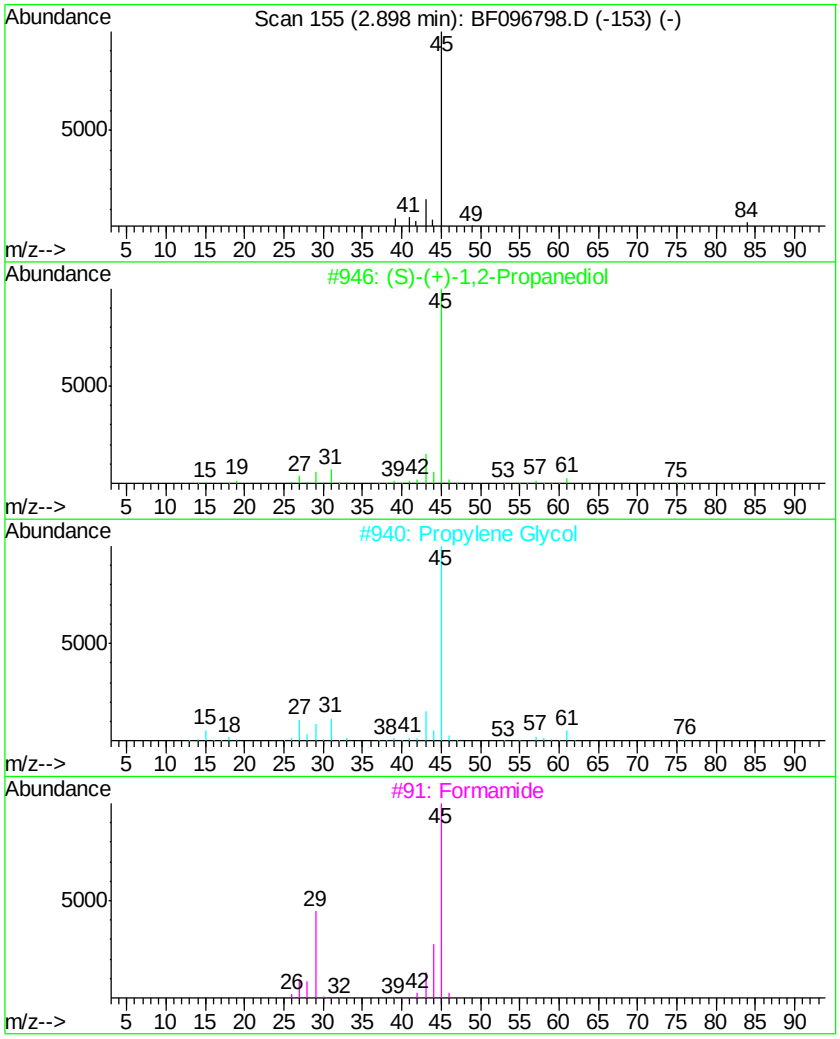
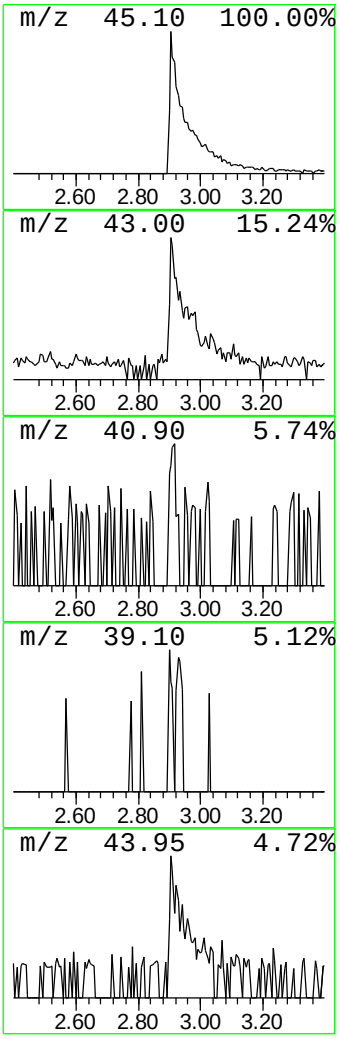
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	2.03 ng	61695	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Formamide	45	CH3NO	000075-12-7	7
4	Ethyl ether	74	C4H10O	000060-29-7	4
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	4





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Operator : SJ/JU
Sample : I4187-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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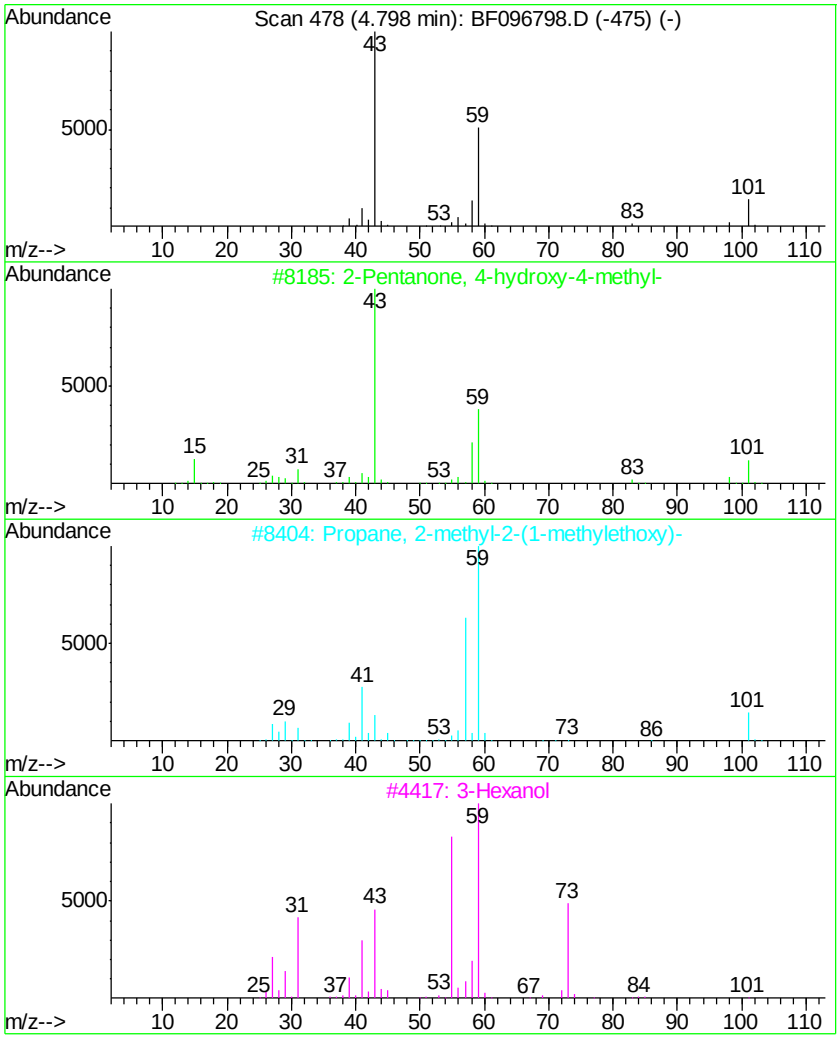
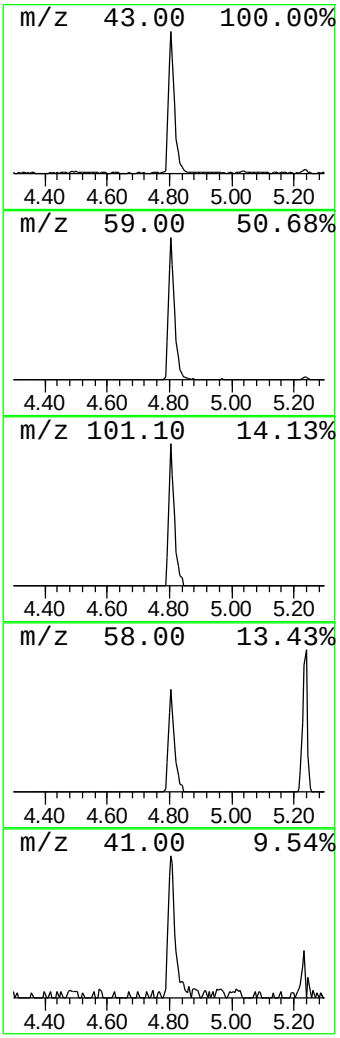
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	9.14 ng	278195	1,4-Dichlorobenzene-d4	6.63

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	102	C6H14O	000623-37-0	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096798.D
Acq On : 15 Jul 2017 3:38
Operator : SJ/JU
Sample : I4187-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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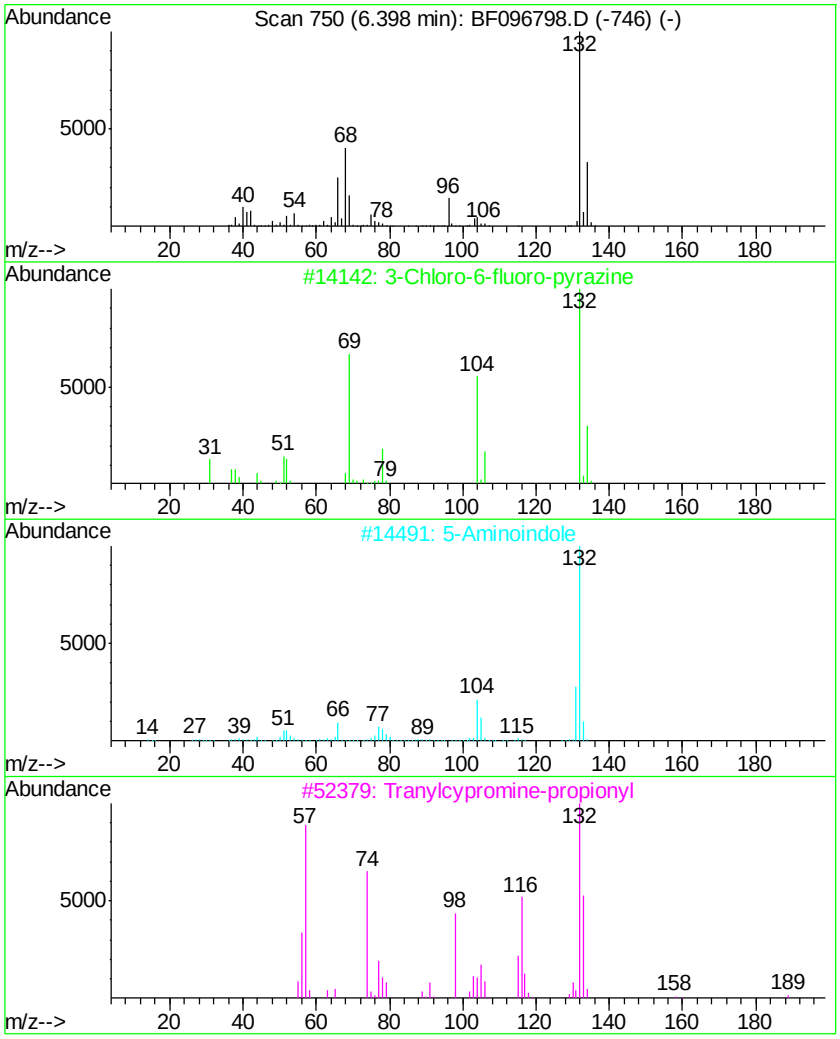
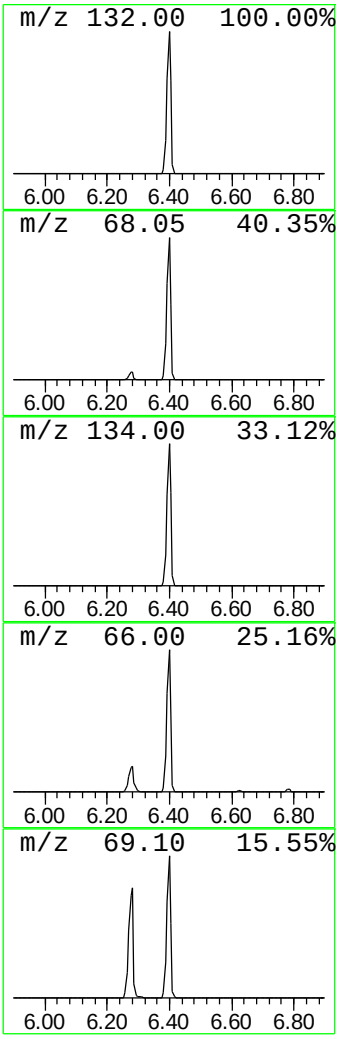
Peak Number 3 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	70.33 ng	2141420	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Sample : I4187-08
Misc :
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Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
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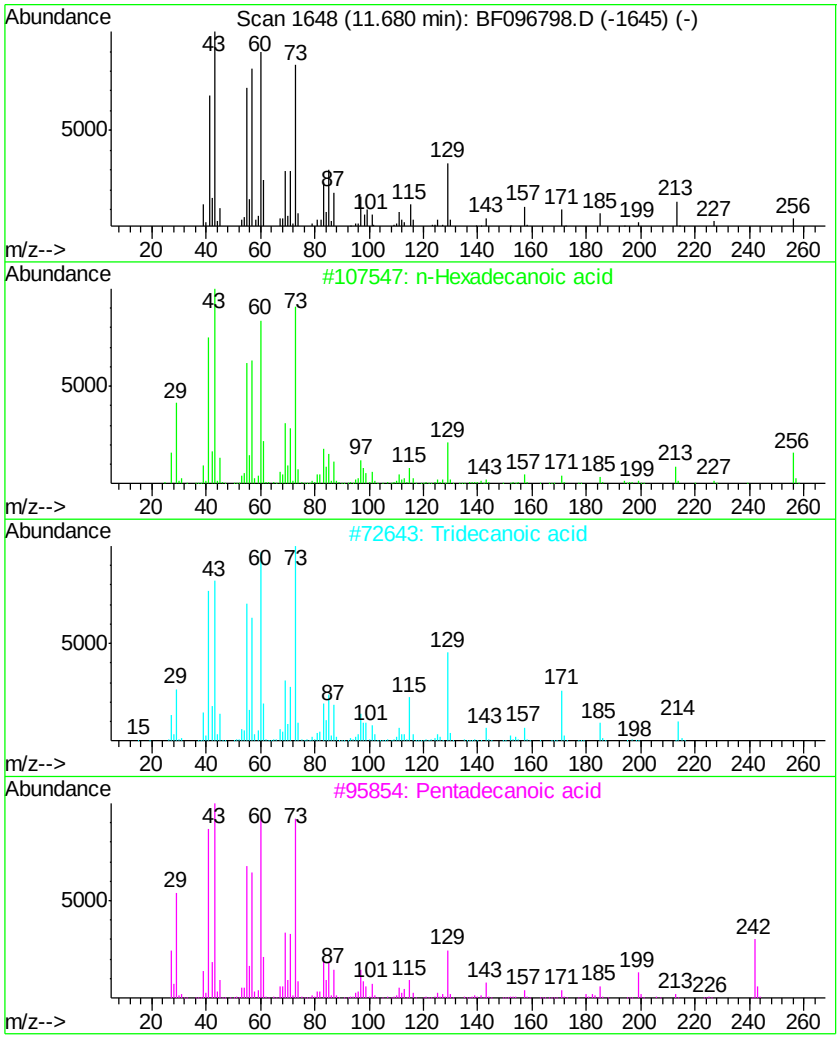
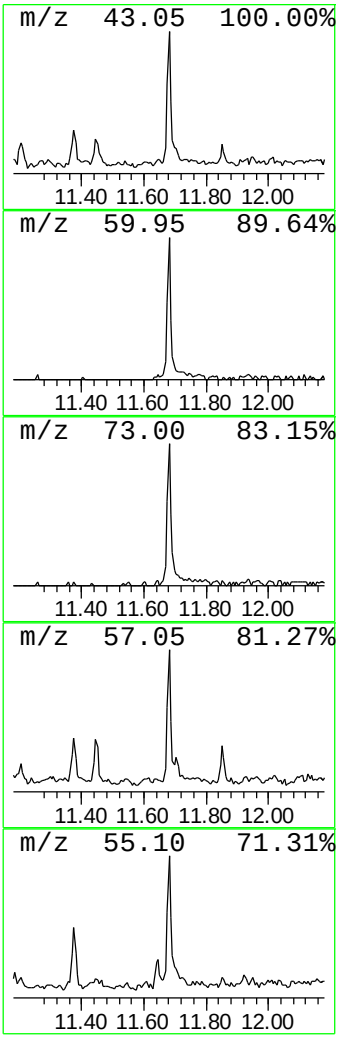
Peak Number 5 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	4.12 ng	122935	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
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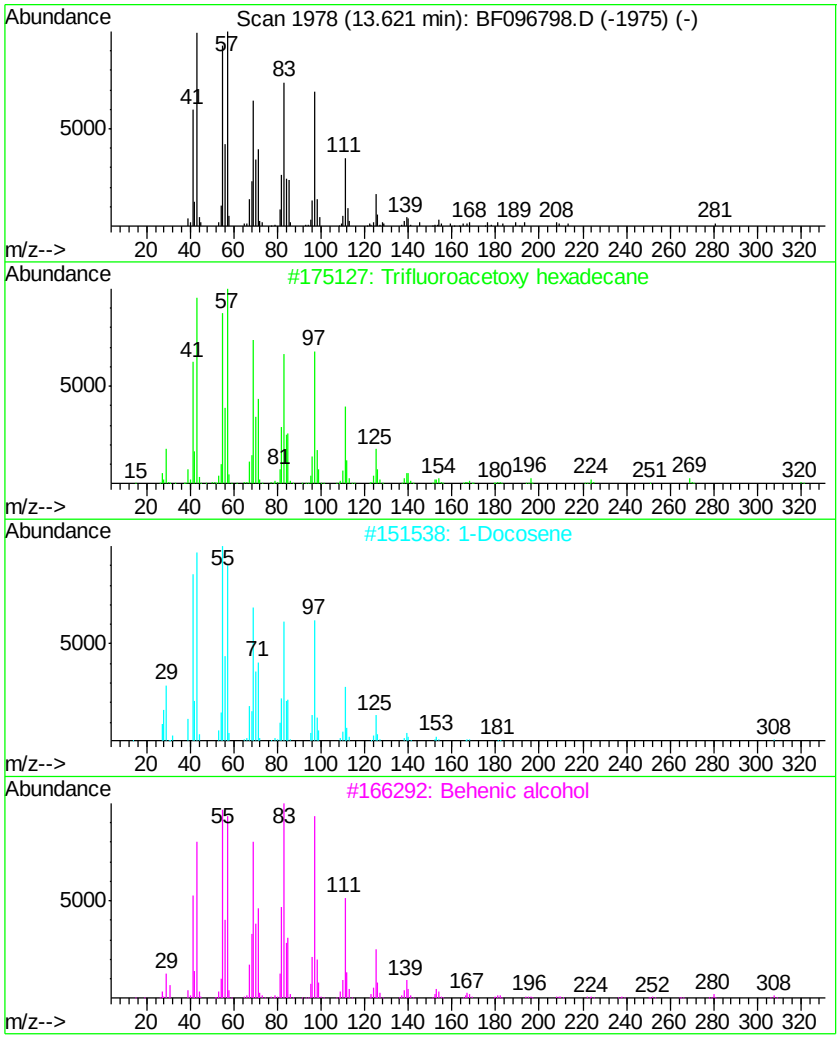
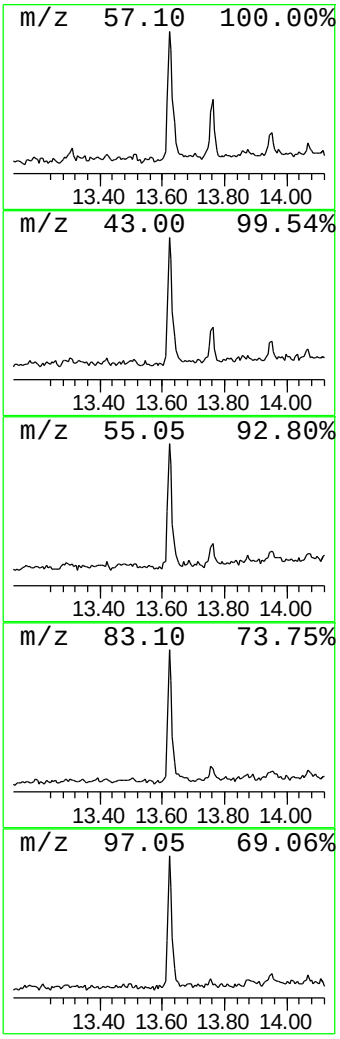
Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	6.22 ng	235305	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Docosene	308	C22H44	001599-67-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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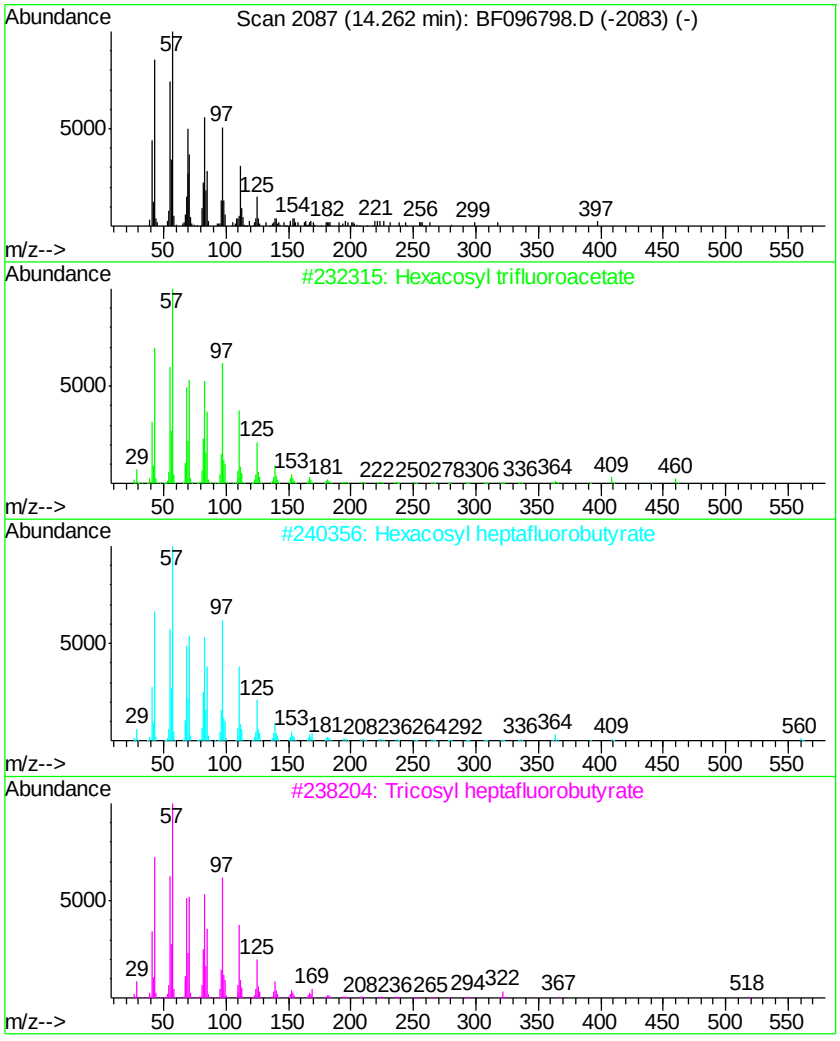
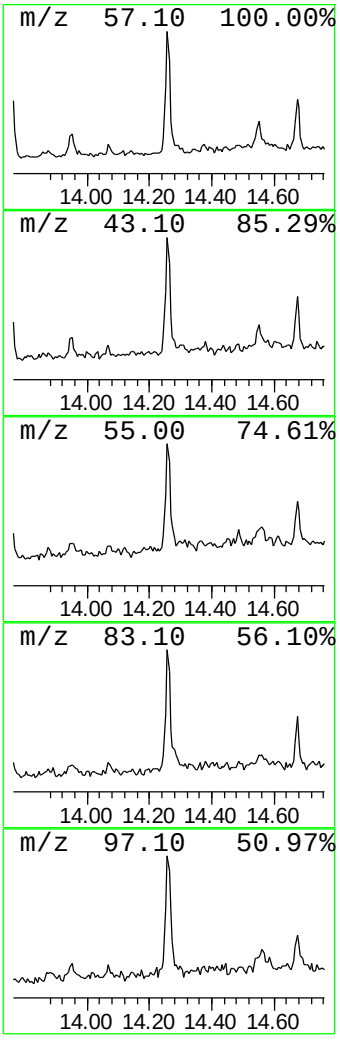
Peak Number 7 Hexacosyl trifluoroacetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	5.91 ng	223430	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
2	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	91





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Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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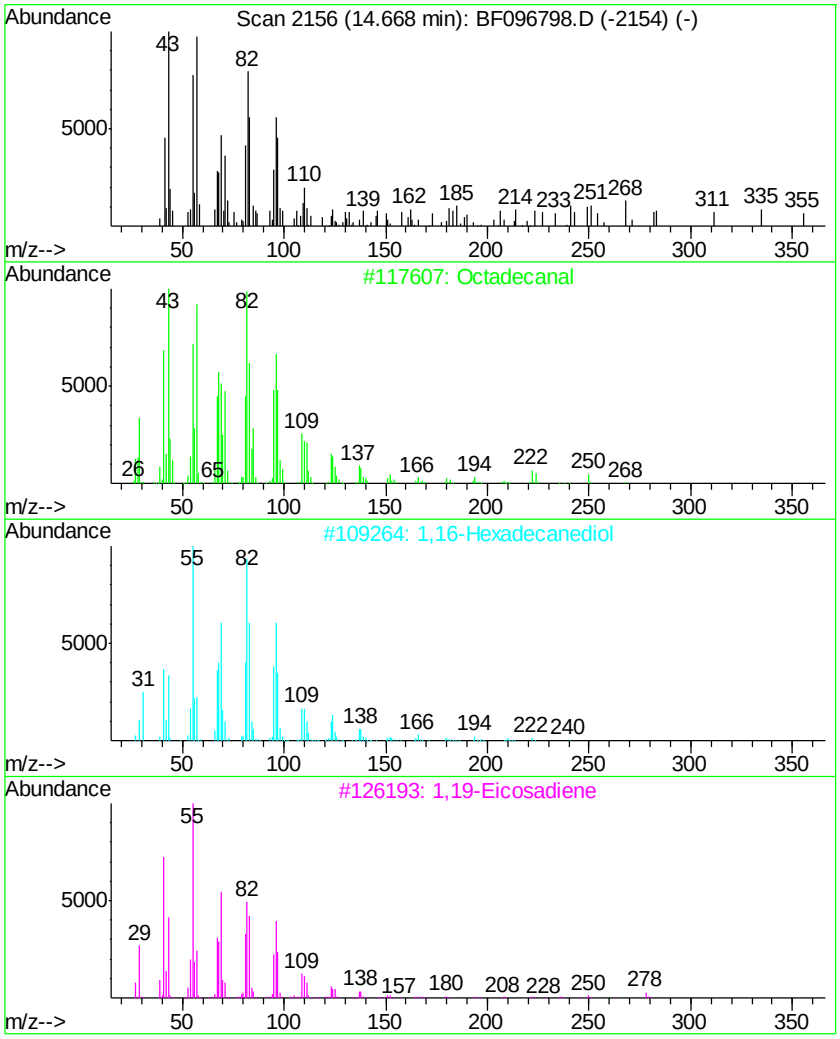
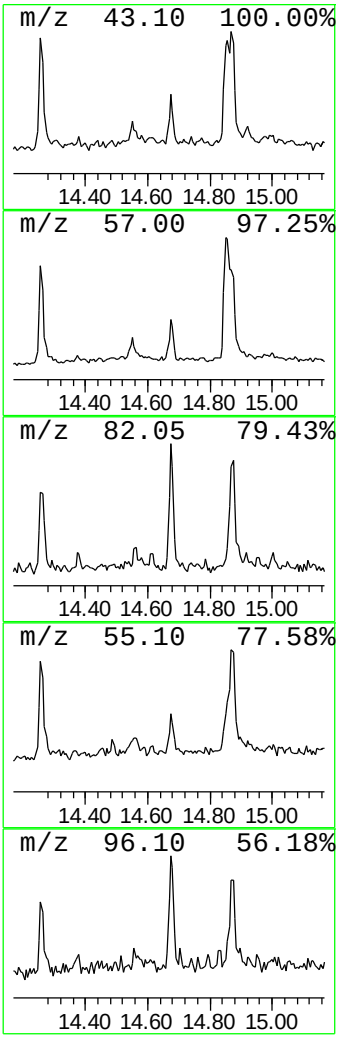
Peak Number 8 Octadecanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	4.05 ng	92415	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	81
2	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	81
3	1,19-Eicosadiene	278	C20H38	014811-95-1	74
4	Octadecanoic acid, 3-hydroxy-2-t...	511	C33H66O3	018951-36-5	72
5	17-Octadecenal	266	C18H34O	056554-86-0	72





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Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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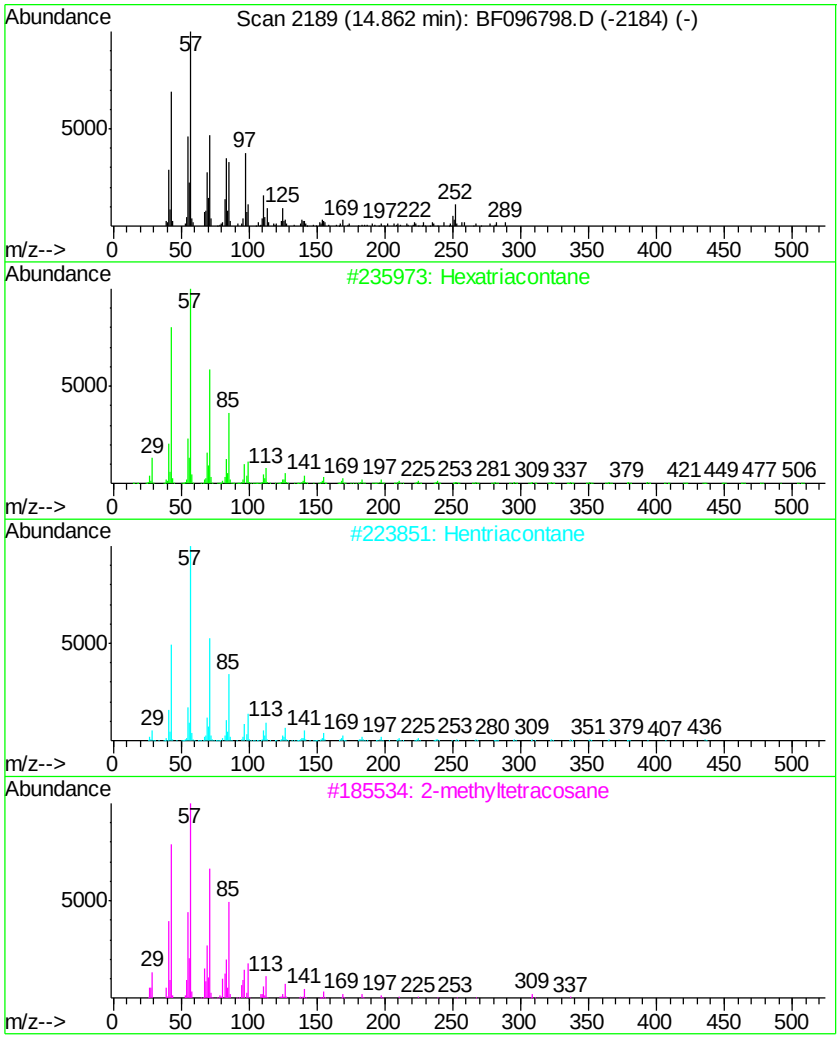
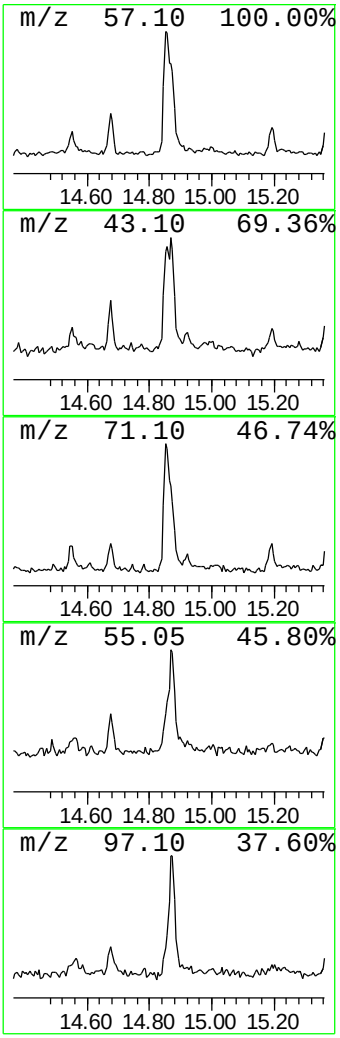
Peak Number 9 Hexatriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	7.65 ng	174540	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	83
2	Hentriacontane	437	C31H64	000630-04-6	80
3	2-methyltetracosane	352	C25H52	1000376-72-6	74
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	72
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096798.D
Acq On : 15 Jul 2017 3:38
Operator : SJ/JU
Sample : I4187-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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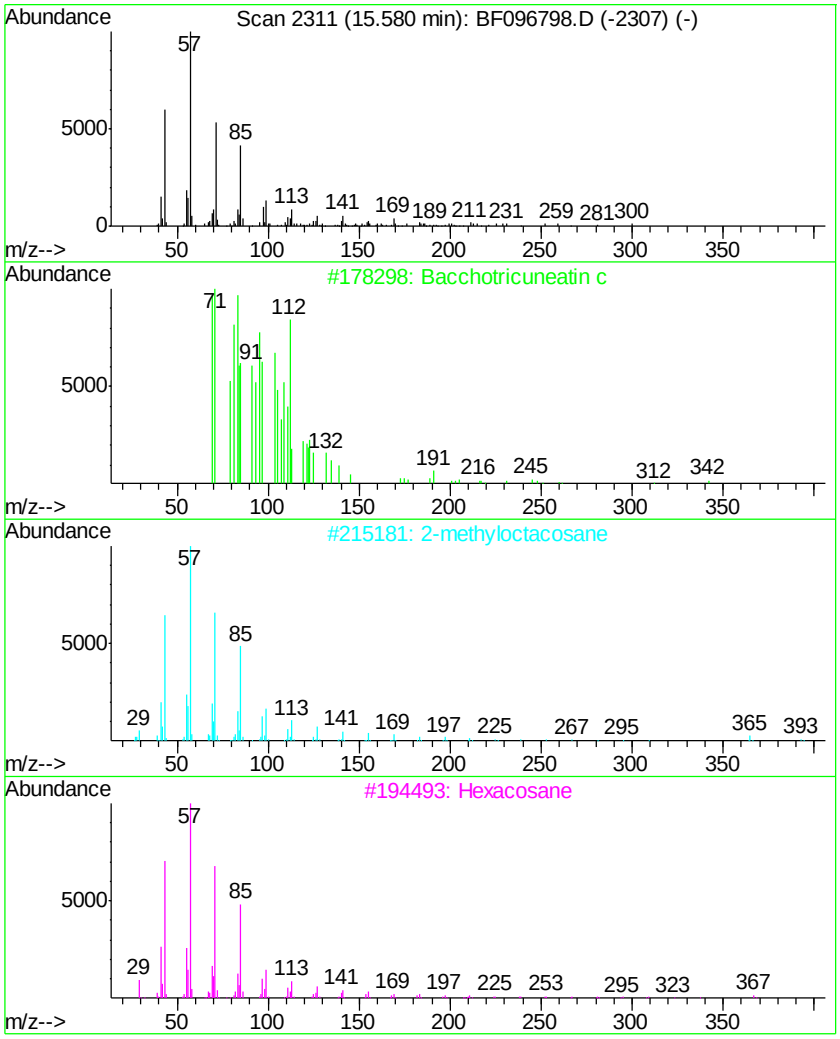
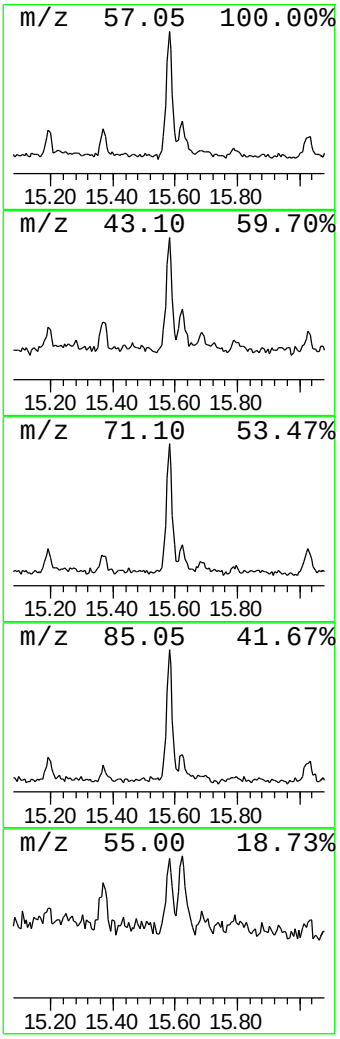
Peak Number 11 Bacchotricuneatin c Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	8.89 ng	202806	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	99
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Octacosane	394	C28H58	000630-02-4	87





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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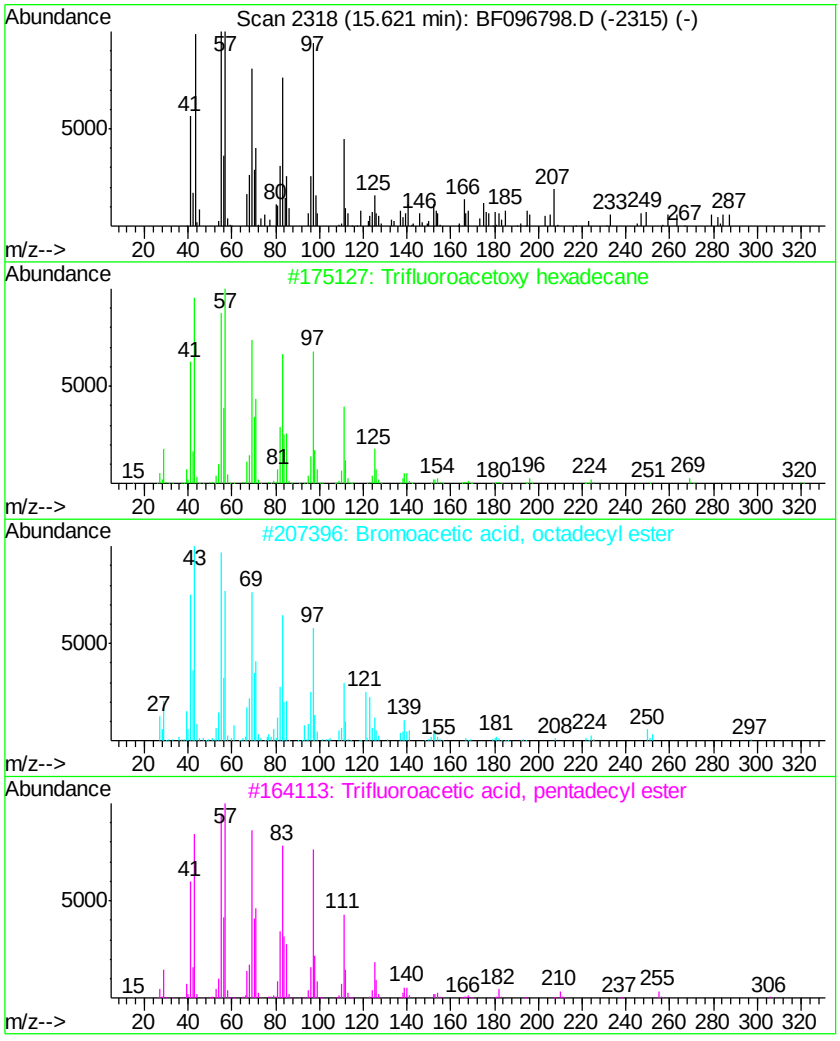
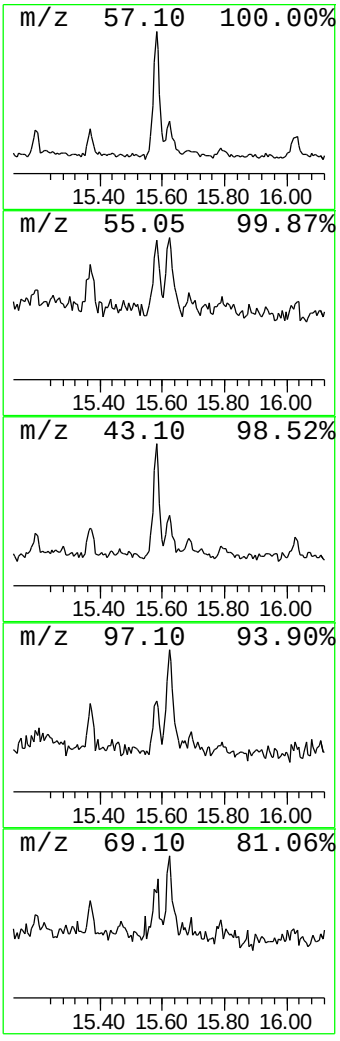
Peak Number 12 Bromoacetic acid, octadecyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	4.61 ng	105043	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	74
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	74
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	64
5	Octacosanol	410	C28H58O	000557-61-9	60





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Data File : BF096798.D
Acq On : 15 Jul 2017 3:38
Operator : SJ/JU
Sample : I4187-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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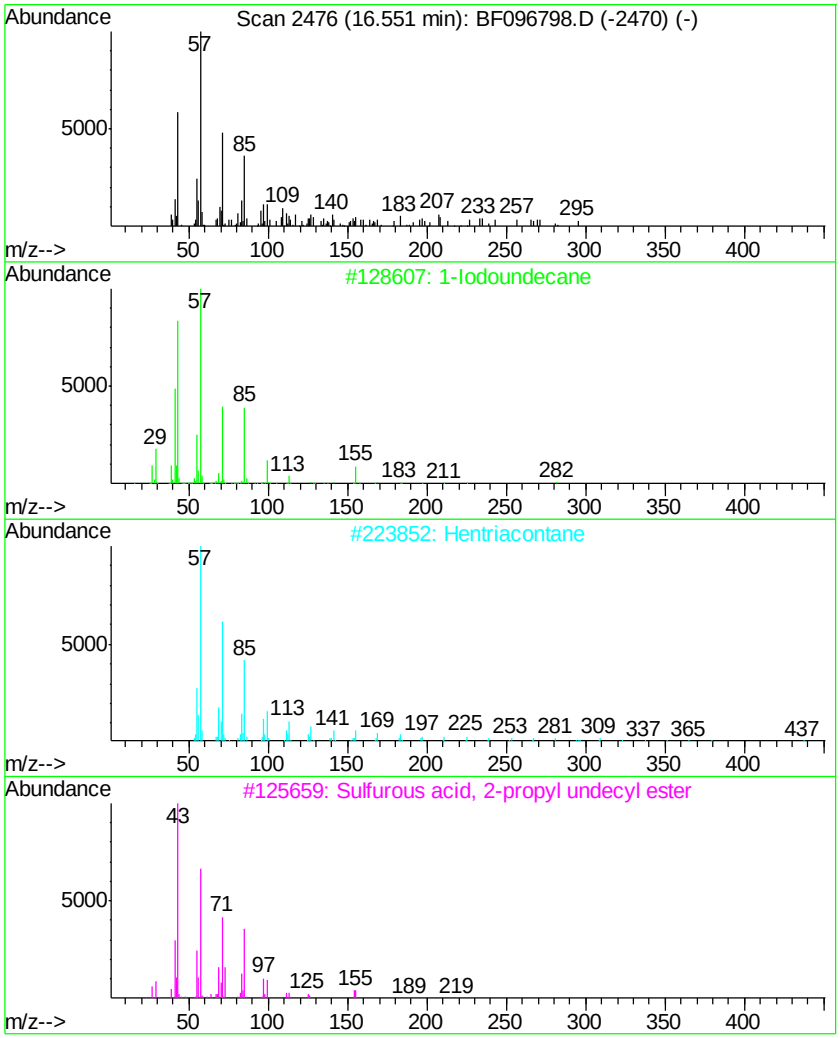
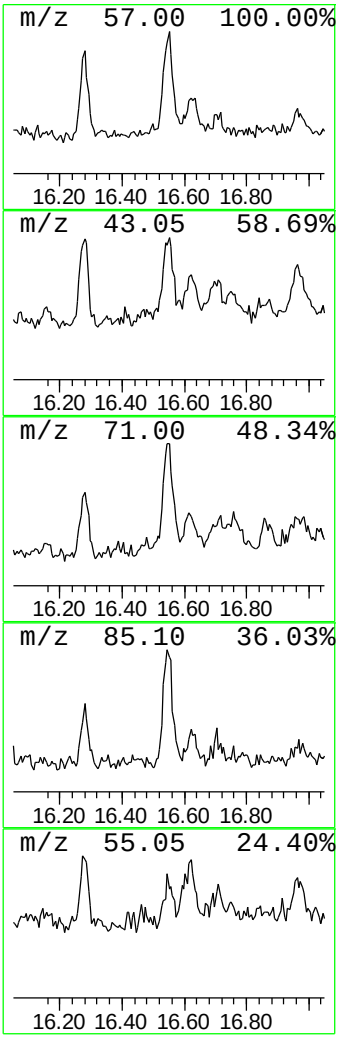
Peak Number 14 1-Iodoundecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	6.11 ng	139415	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodoundecane	282	C11H23I	004282-44-4	70
2	Hentriacontane	437	C31H64	000630-04-6	62
3	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	59
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	58
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58





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Data File : BF096798.D
Acq On : 15 Jul 2017 3:38
Operator : SJ/JU
Sample : I4187-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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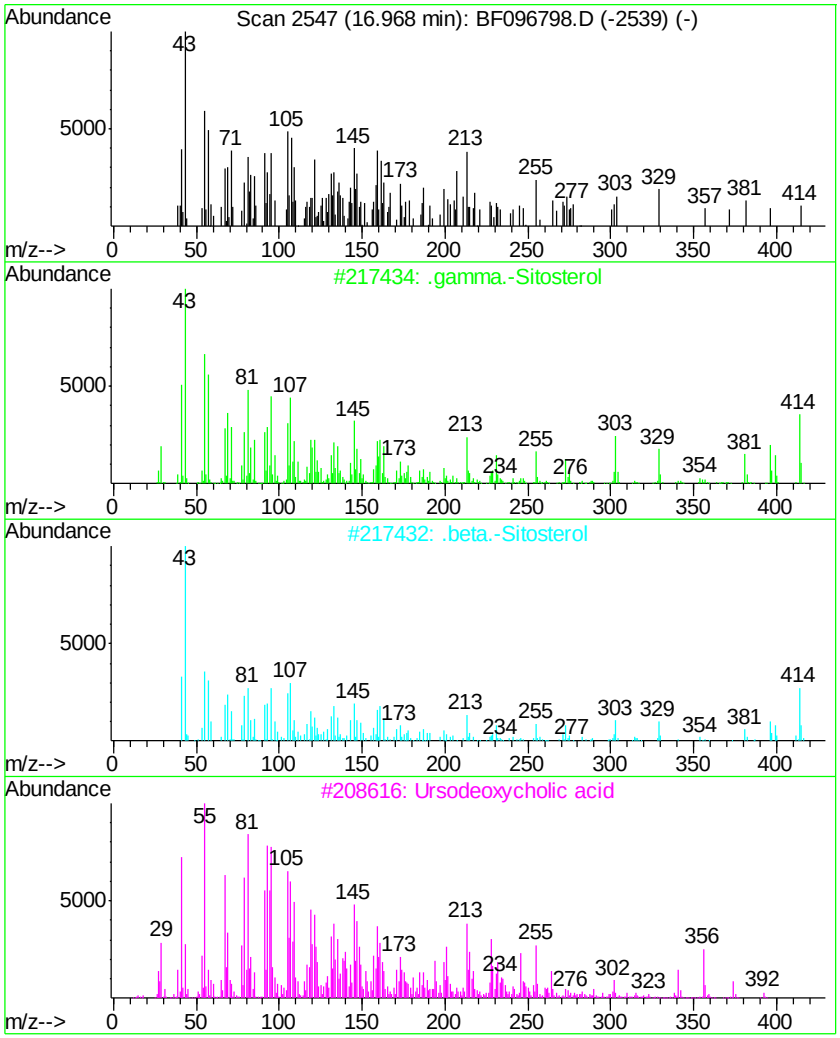
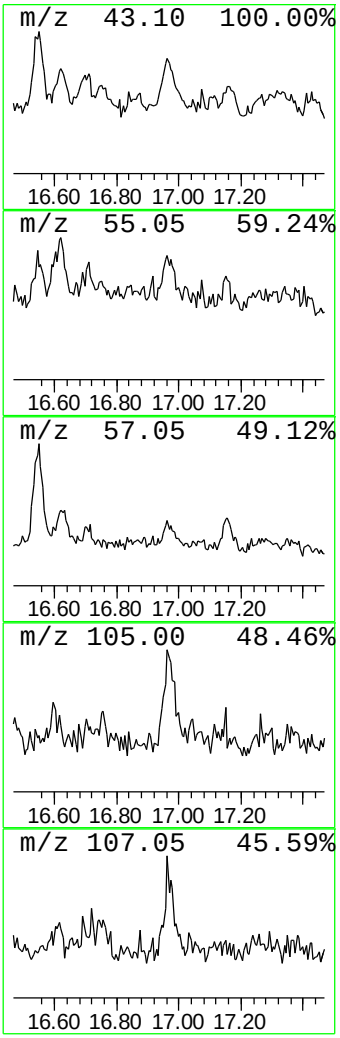
Peak Number 15 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	10.65 ng	242974	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	93
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	56
3	Ursodeoxycholic acid	392	C24H40O4	000128-13-2	12
4	26,27-Dinorcholesta-5,22-dien-3-...	356	C25H40O	057597-10-1	10
5	Methandriol	304	C20H32O2	000521-10-8	10





Tentatively Identified Compound (LSC) summary

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Data File : BF096798.D
Acq On : 15 Jul 2017 3:38
Operator : SJ/JU
Sample : I4187-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB8-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	2.90	2.0	ng	61695	1	6.63	608987	20.0
2-Pentanone, 4-hy...	4.80	9.1	ng	278195	1	6.63	608987	20.0
unknown6.40	6.40	70.3	ng	2141420	1	6.63	608987	20.0
n-Hexadecanoic acid	11.68	4.1	ng	122935	4	11.13	597095	20.0
Trifluoroacetoxy ...	13.62	6.2	ng	235305	5	13.76	756165	20.0
Hexacosyl trifluo...	14.26	5.9	ng	223430	5	13.76	756165	20.0
Octadecanal	14.67	4.0	ng	92415	6	15.14	456141	20.0
Hexatriacontane	14.86	7.7	ng	174540	6	15.14	456141	20.0
Bacchotricuneatin c	15.58	8.9	ng	202806	6	15.14	456141	20.0
Bromoacetic acid,...	15.62	4.6	ng	105043	6	15.14	456141	20.0
1-Iodoundecane	16.55	6.1	ng	139415	6	15.14	456141	20.0
.gamma.-Sitosterol	16.97	10.7	ng	242974	6	15.14	456141	20.0