LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101523.D
Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

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-BF121417.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	5.028	496	500	517	rBV	469327	683631	22.81%	2.244%
2	5.434	565	569	591	rBV	2476785	2783695	92.89%	9.137%
3	6.451	738	742	760	rBV	2510618	2864476	95.59%	9.402%
4	6.581	760	764	779	rVB	2857358	2703260	90.21%	8.873%
5	6.810	799	803	811	rBV	825764	823248	27.47%	2.702%
6	6.963	825	829	844	rVB	2318798	2188580	73.03%	7.183%
7	7.375	895	899	917	rBV	1693307	1798413	60.01%	5.903%
8	8.092	1017	1021	1037	rBV	983901	1087444	36.29%	3.569%
9	9.163	1199	1203	1212	rBV	3189200	2996696	100.00%	9.836%
10	9.563	1264	1271	1277	rBV	147867	159812	5.33%	0.525%
11	9.763	1300	1305	1309	rBV	62528	49659	1.66%	0.163%
12	9.810	1309	1313	1315	rBV	34259	33138	1.11%	0.109%
13	9.845	1315	1319	1327	rVV2	1233286	1125590	37.56%	3.694%
14	10.263	1387	1390	1393	rVB	75286	58654	1.96%	0.193%
15	10.639	1450	1454	1468	rBV	1472555	1613122	53.83%	5.295%
16	10.733	1468	1470	1479	rVB	61482	68541	2.29%	0.225%
17	11.339	1569	1573	1582	rBV	1162514	1179361	39.36%	3.871%
18	11.851	1656	1660	1671	rBV4	74450	106739	3.56%	0.350%
19	12.557	1777	1780	1784	rBV	114157	105595	3.52%	0.347%
20	12.639	1791	1794	1803	rBV2	50939	65005	2.17%	0.213%
21	12.786	1813	1819	1823	rBV	87139	106194	3.54%	0.349%
22	12.921	1837	1842	1845	rBV	2526800	2302719	76.84%	7.558%
23	13.116	1871	1875	1877	rBV	60211	71867	2.40%	0.236%
24	13.468	1931	1935	1938	rBV4	26289	33499	1.12%	0.110%
25	13.798	1988	1991	1999	rBV	397136	509318	17.00%	1.672%
26	13.939	2011	2015	2019	rBV	32691	37403	1.25%	0.123%
27	13.986	2019	2023	2027	rBV	791411	768206	25.64%	2.521%
28	14.121	2043	2046	2057	rVB6	25293	49327	1.65%	0.162%
29	14.439	2094	2100	2106	rBV3	166100	318916	10.64%	1.047%
30	14.721	2145	2148	2152	rBV2	36277	42876	1.43%	0.141%
31	14.798	2159	2161	2165	rVB	32167	31522	1.05%	0.103%
32	14.868	2170	2173	2180	rVB3	65278	73485	2.45%	0.241%
33	15.057	2198	2205	2208	rBV	574094	669115	22.33%	2.196%
34	15.086	2208	2210	2215	rVV2	86374	130512	4.36%	0.428%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101523.D
Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.139	2217	2219	2223	rVB3	35061	32390	1.08%	0.106%
36	15.404	2261	2264	2265	rBV	27826	32002	1.07%	0.105%
37	15.457	2269	2273	2282	rVB	571823	764739	25.52%	2.510%
38	15.627	2298	2302	2308	rBV2	116959	152702	5.10%	0.501%
39	15.851	2335	2340	2345	rVB	391331	560065	18.69%	1.838%
40	15.909	2346	2350	2357	rBV3	73634	143131	4.78%	0.470%
41	16.086	2378	2380	2385	rBV3	31888	40877	1.36%	0.134%
42	16.633	2467	2473	2482	rVB	193360	354801	11.84%	1.165%
43	16.915	2518	2521	2532	rVB5	63223	147618	4.93%	0.485%
44	17.021	2535	2539	2548	rBV8	52840	131264	4.38%	0.431%
45	17.433	2604	2609	2618	rBV10	87879	215632	7.20%	0.708%
46	18.303	2752	2757	2765	rVB7	105978	252845	8.44%	0.830%

Sum of corrected areas: 30467684

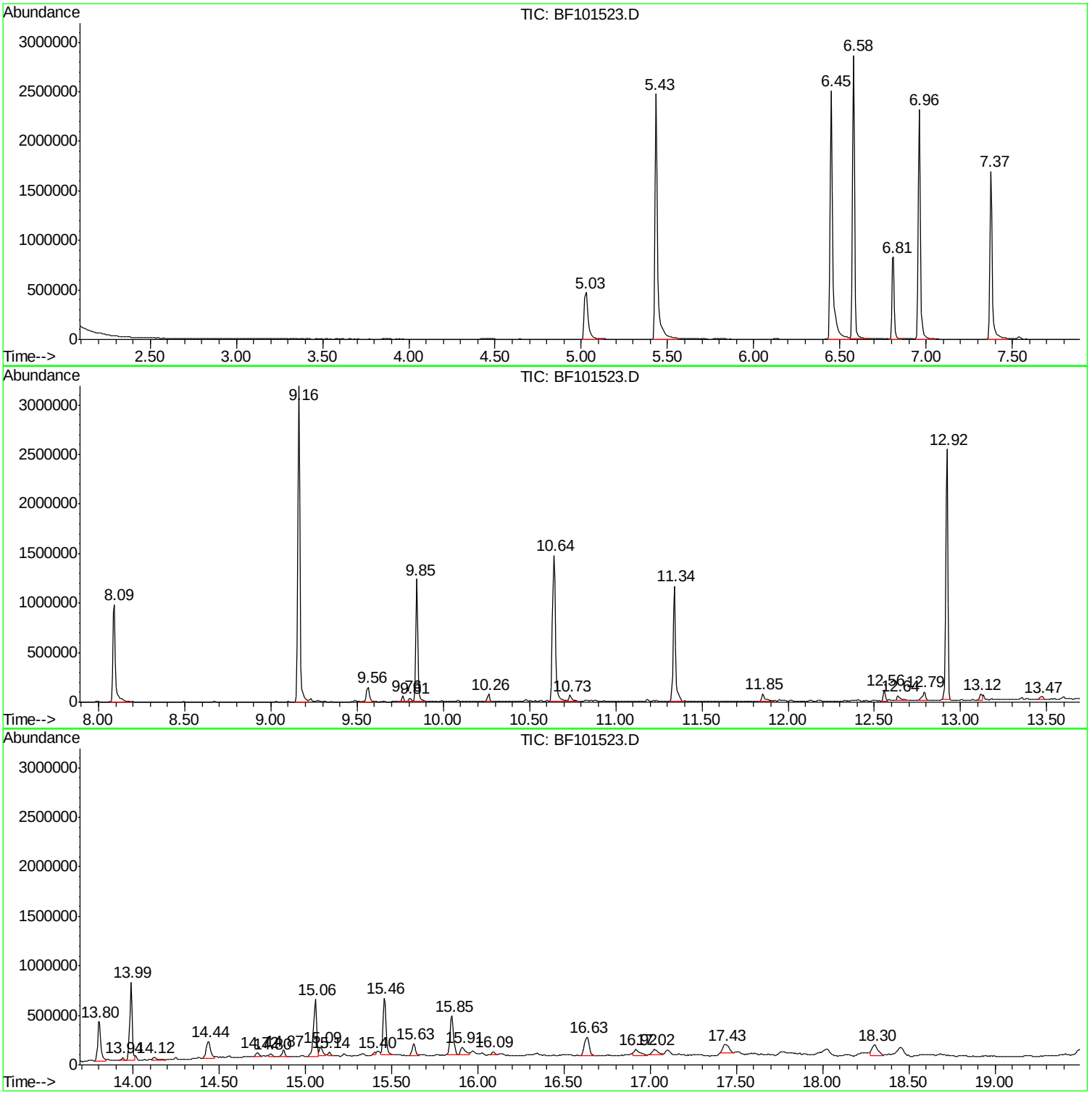
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101523.D
Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101523.D
Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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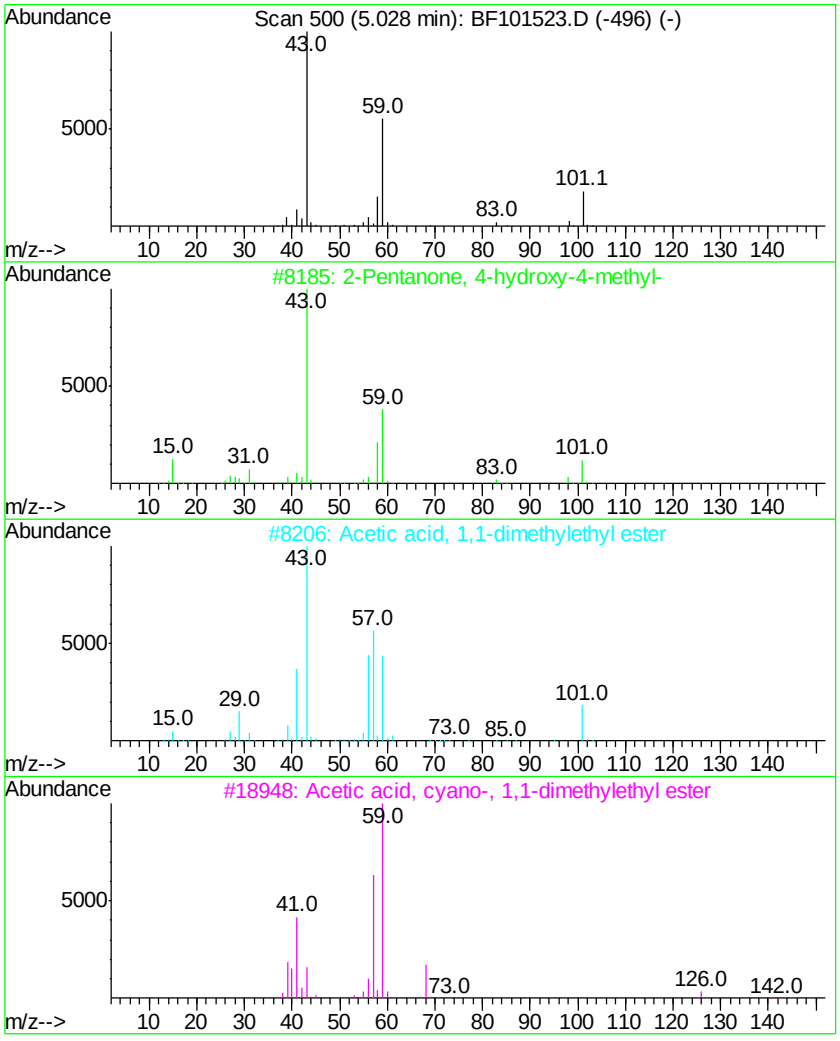
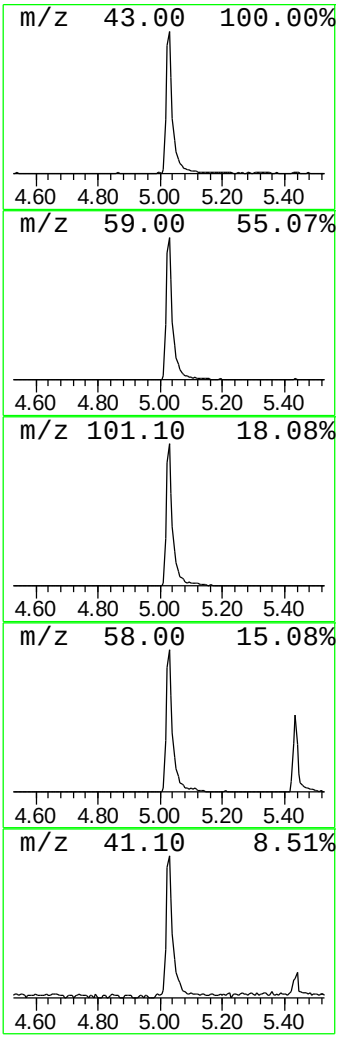
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	16.61 ng	683631	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101523.D
Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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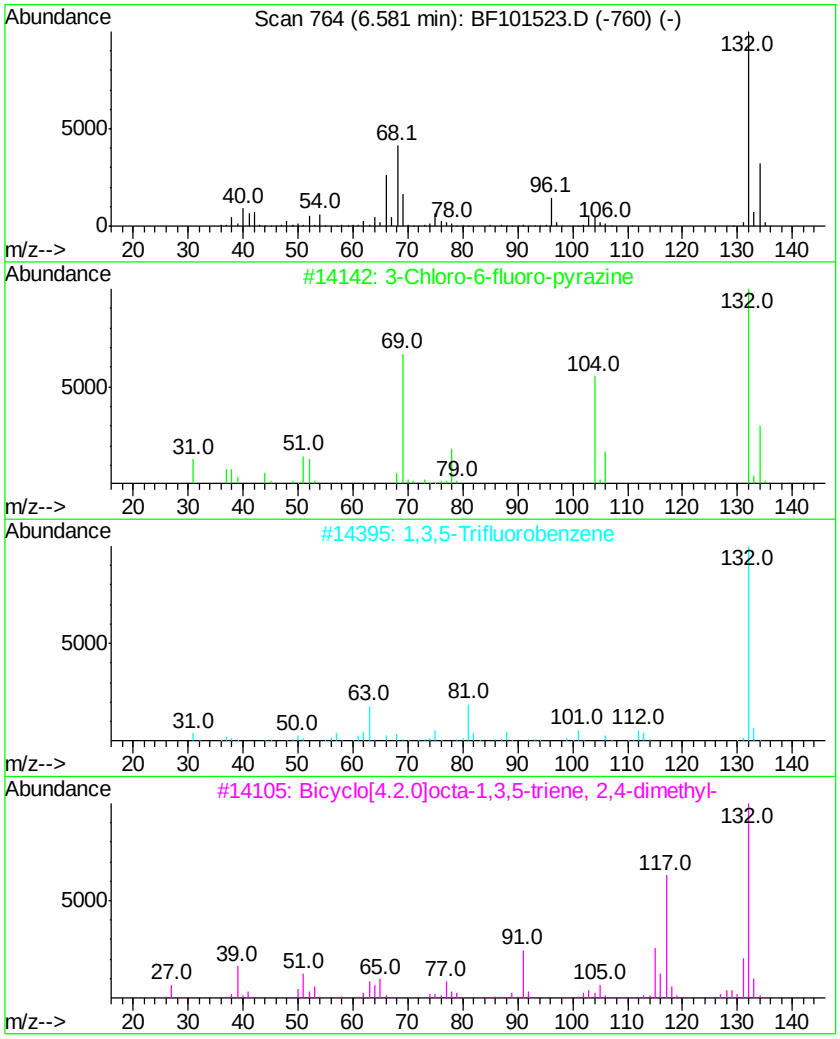
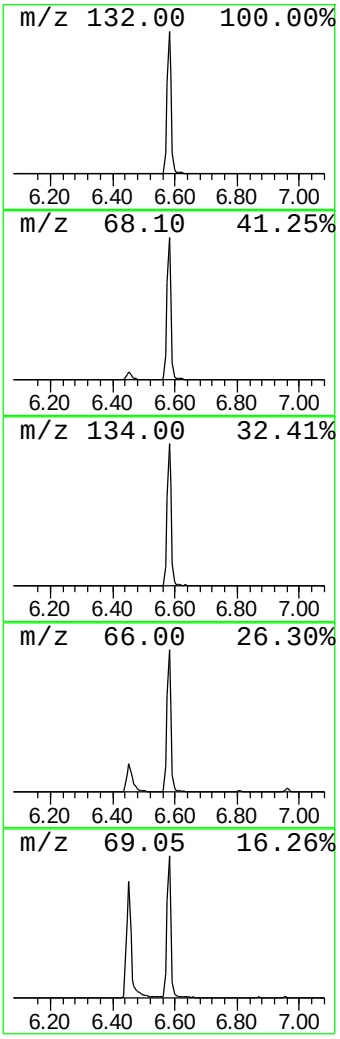
Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	65.67 ng	2703260	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Data File : BF101523.D
Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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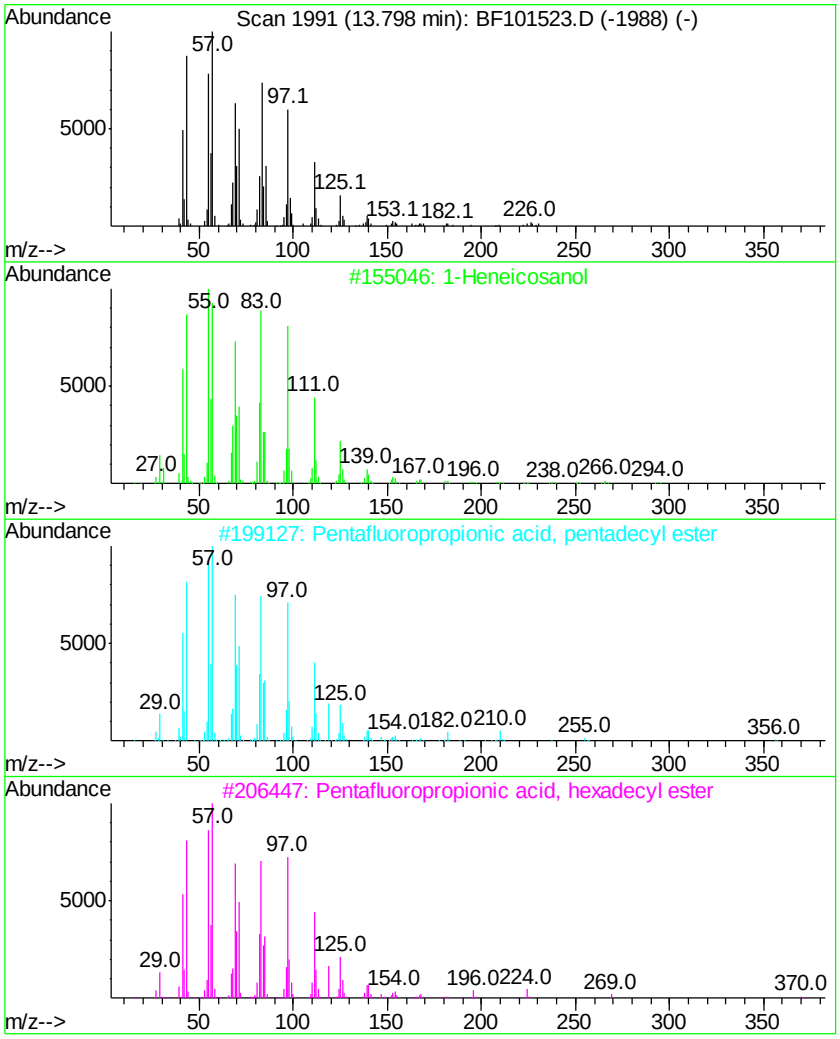
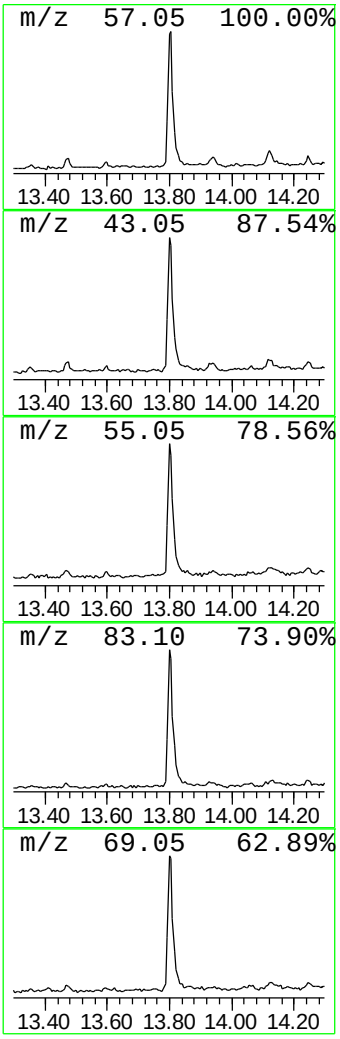
Peak Number 5 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	13.26 ng	509318	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





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Misc :
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Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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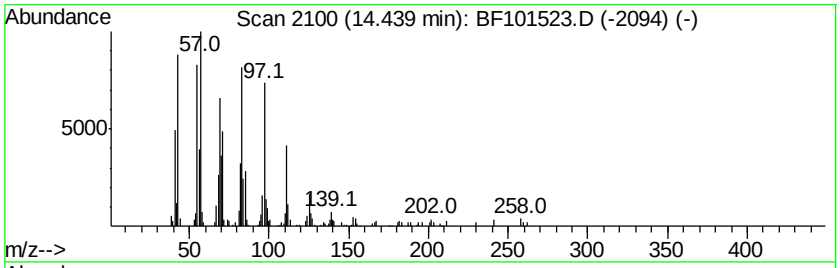
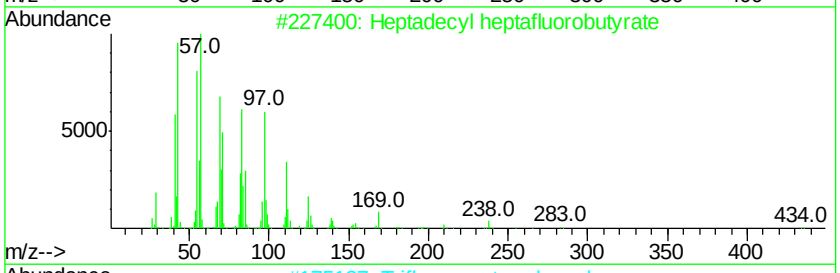
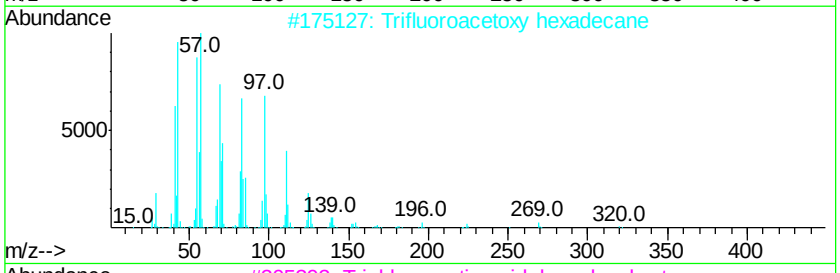
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 8

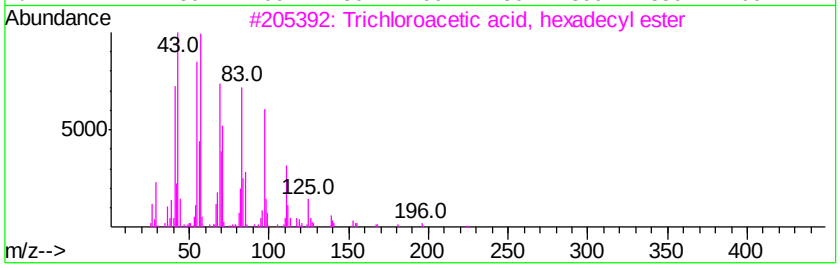
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	8.30 ng	318916	Chrysene-d12	13.99

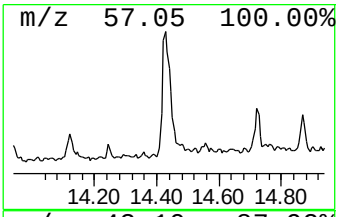
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93

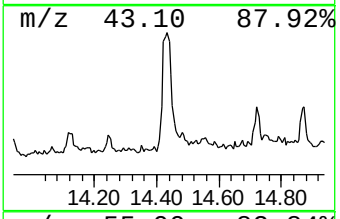


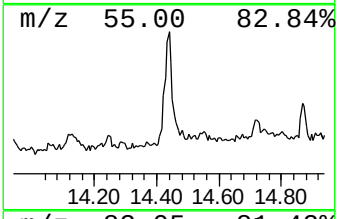


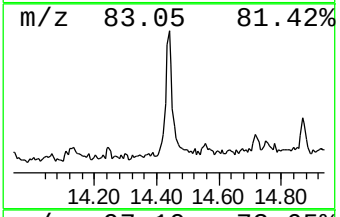


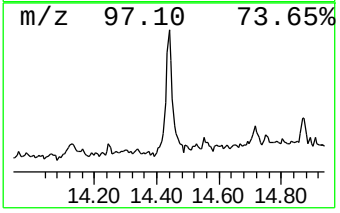












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Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

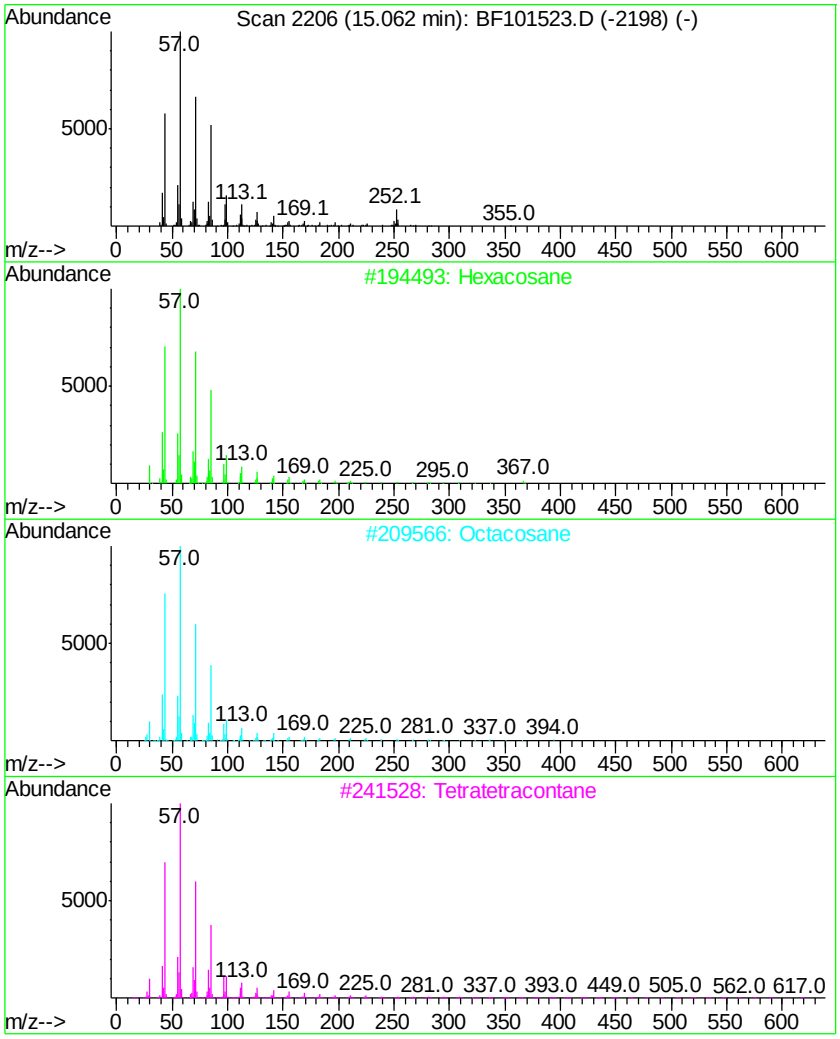
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

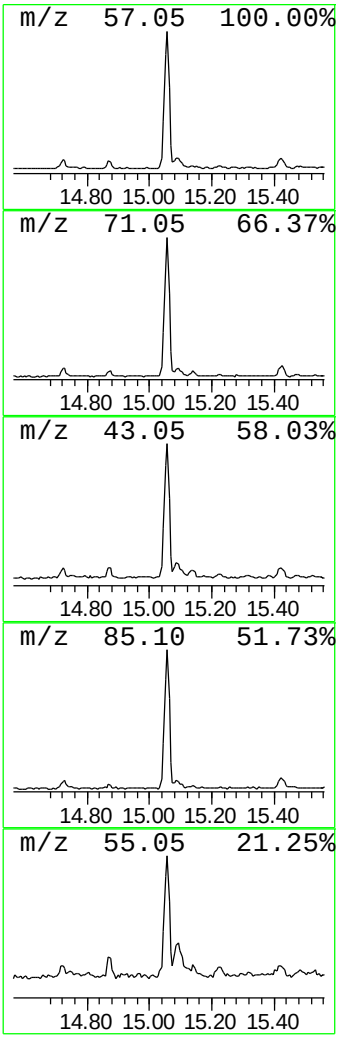
****

Peak Number 7 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	17.50 ng	669115	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Heneicosane	296	C21H44	000629-94-7	87
5	Eicosane	282	C20H42	000112-95-8	87





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101523.D
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Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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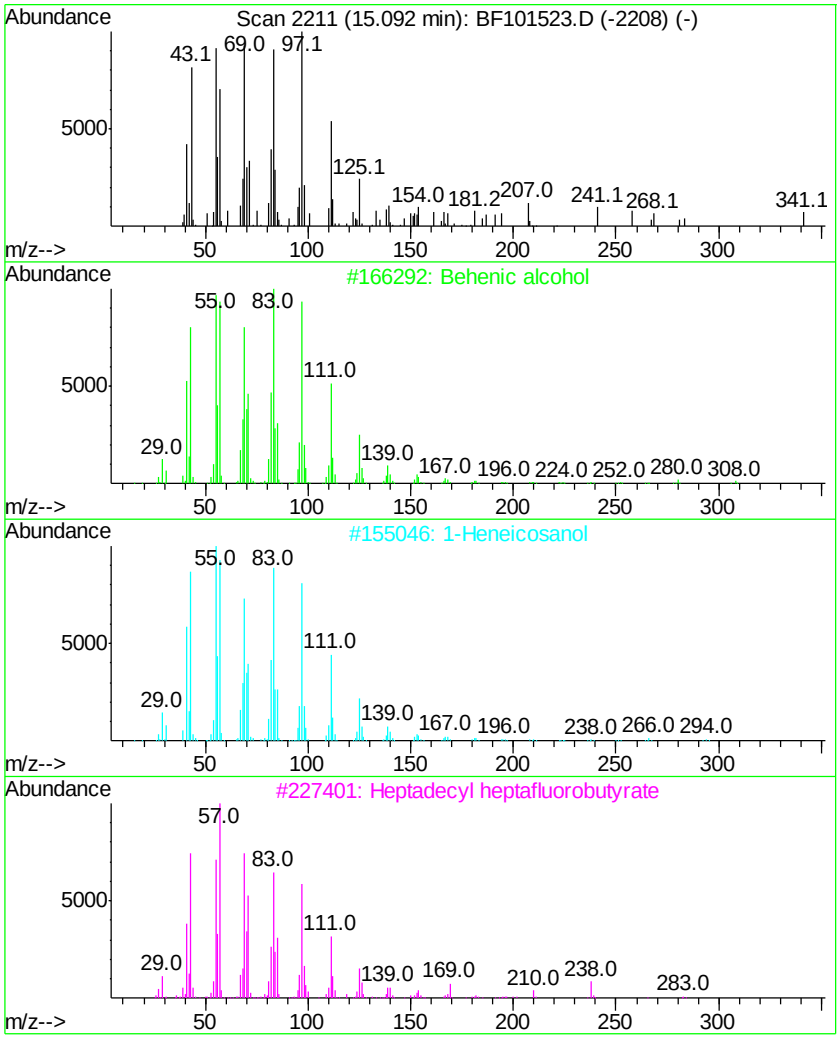
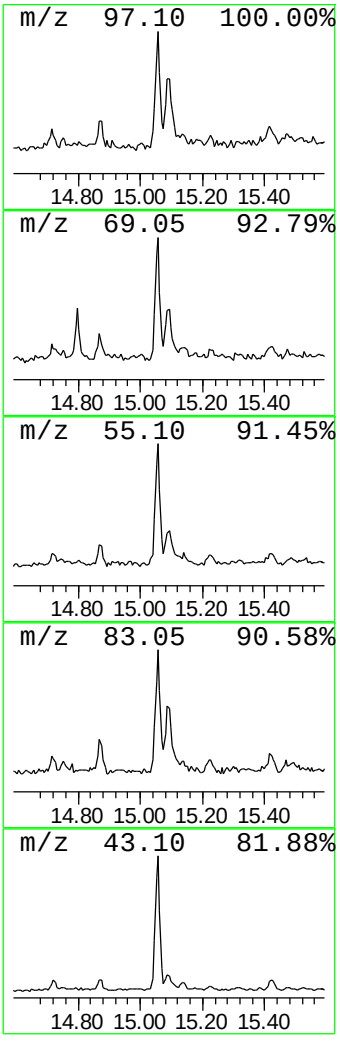
Peak Number 8 Behenic alcohol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.41 ng	130512	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	1-Heneicosanol	312	C21H44O	015594-90-8	80
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	80
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	74
5	1-Nonadecene	266	C19H38	018435-45-5	64





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Data File : BF101523.D
Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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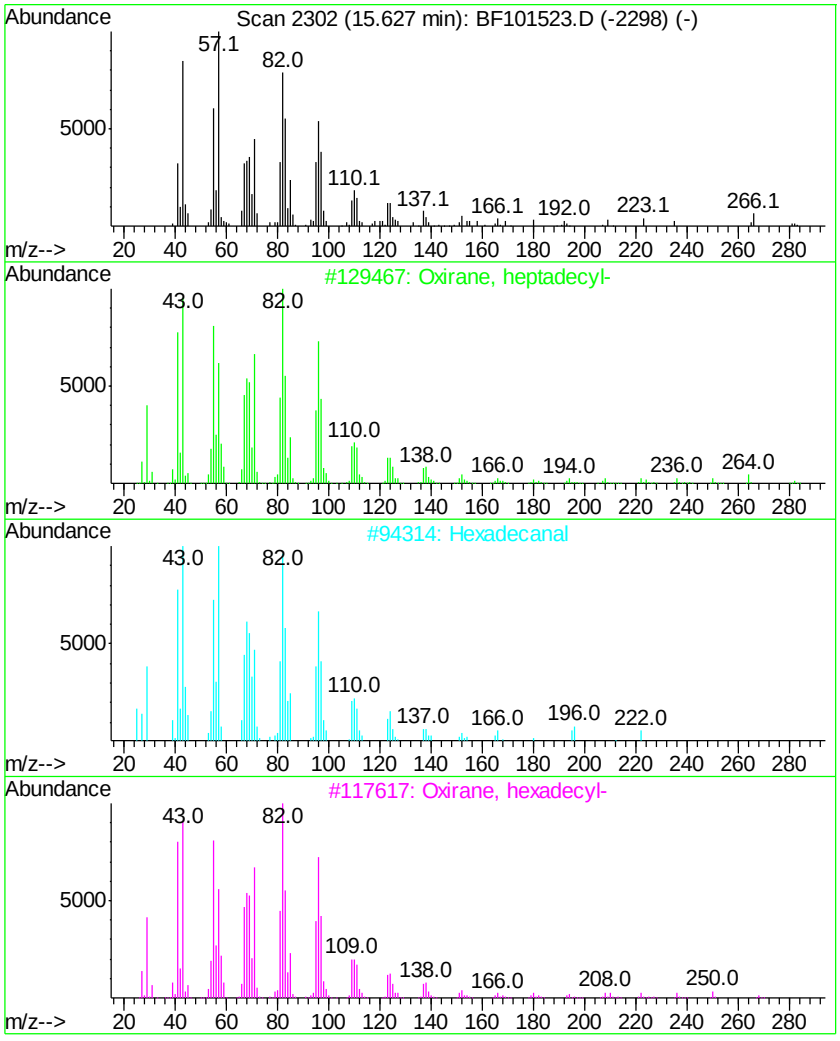
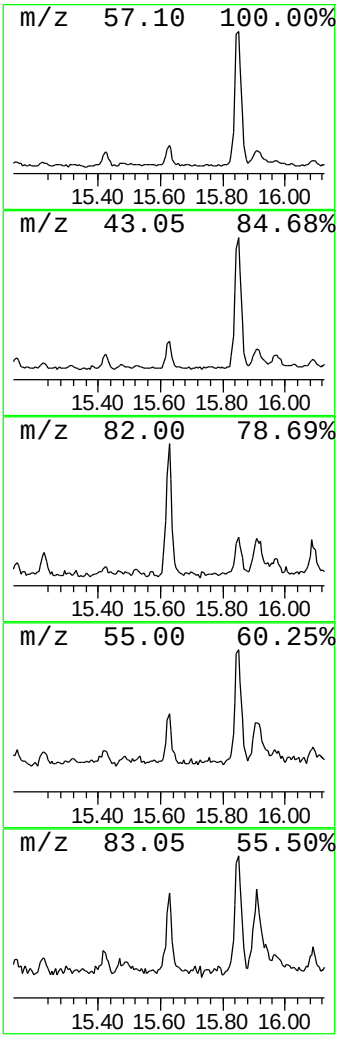
Peak Number 9 Oxirane, heptadecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	3.99 ng	152702	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Hexadecanal	240	C16H32O	000629-80-1	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4	Octadecanal	268	C18H36O	000638-66-4	87
5	1,19-Eicosadiene	278	C20H38	014811-95-1	81





Library Search Compound Report

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Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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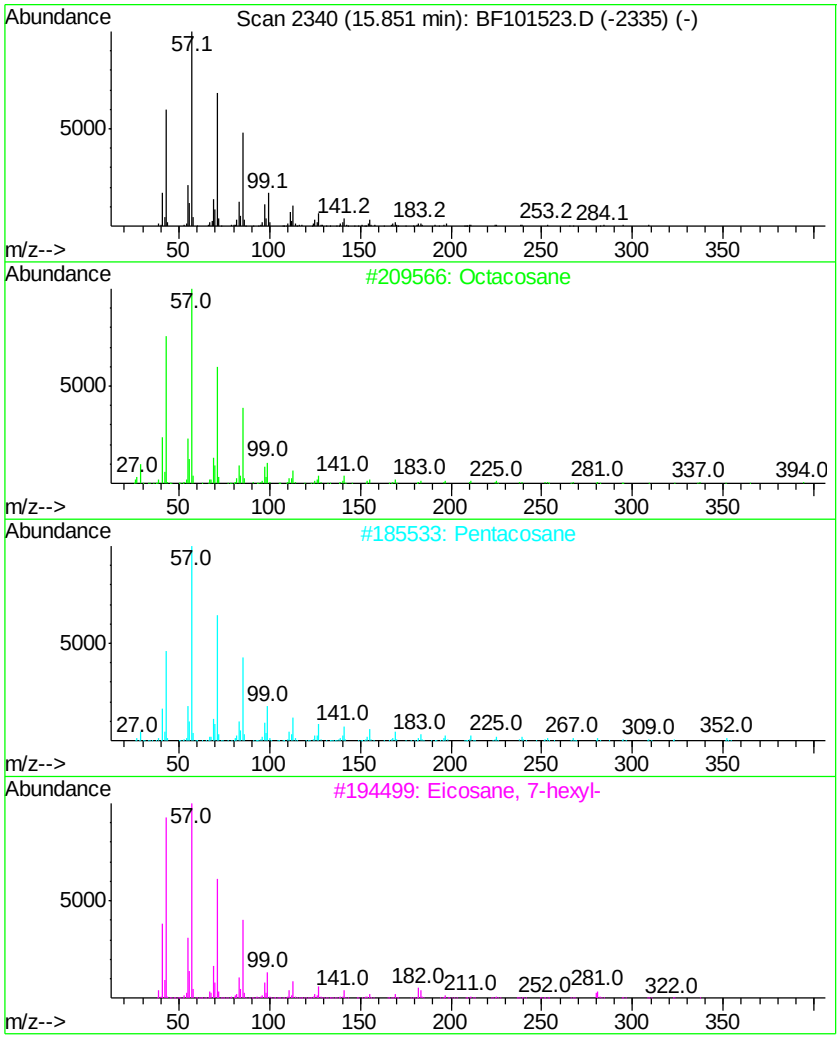
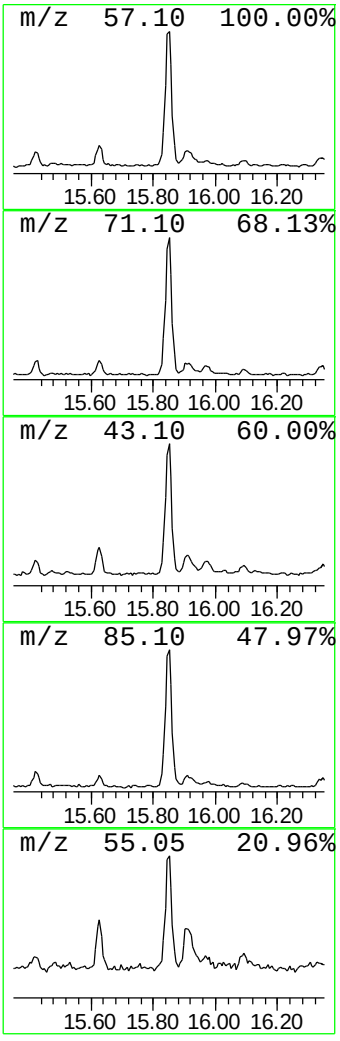
Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	14.65 ng	560065	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	90
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87





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ClientSampleId : 4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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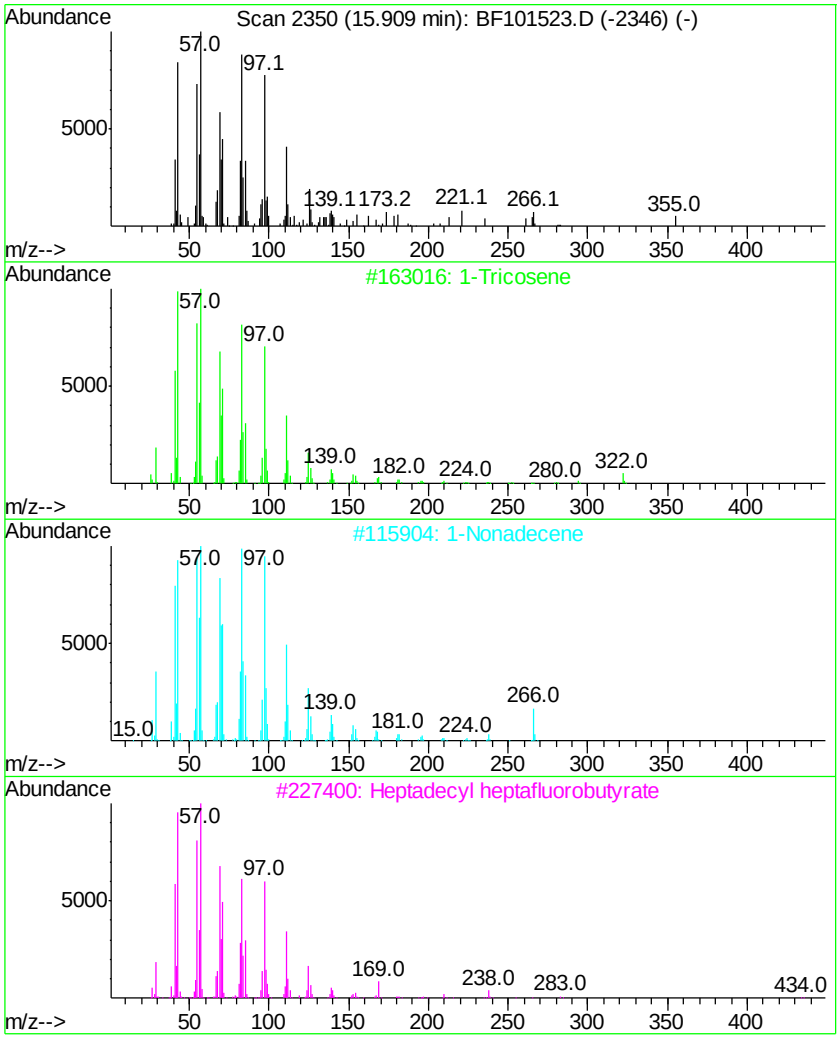
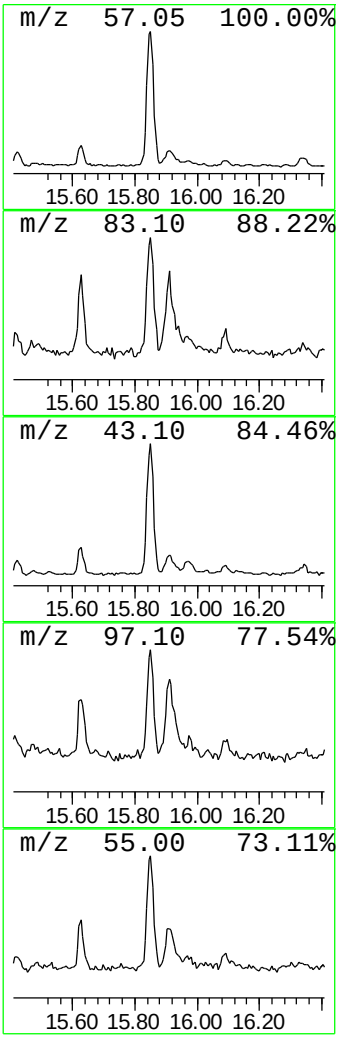
Peak Number 11 1-Tricosene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	3.74 ng	143131	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4	Cyclotetracosane	336	C24H48	000297-03-0	87
5	9-Nonadecene	266	C19H38	031035-07-1	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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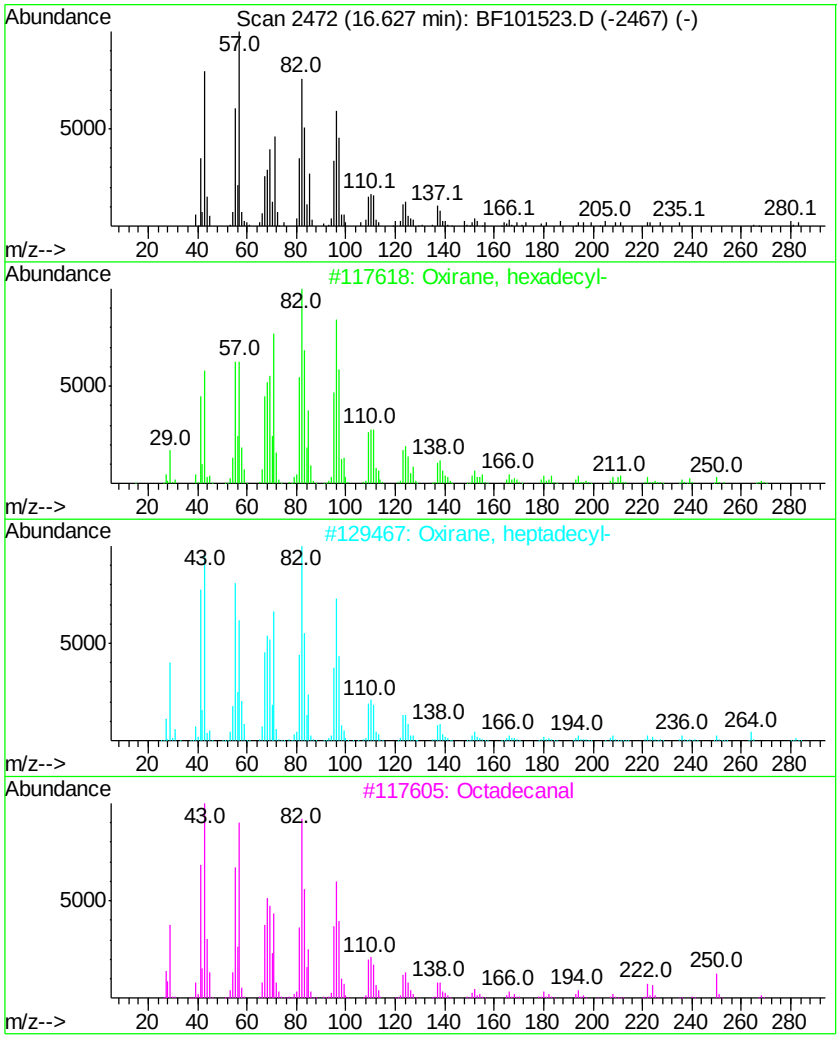
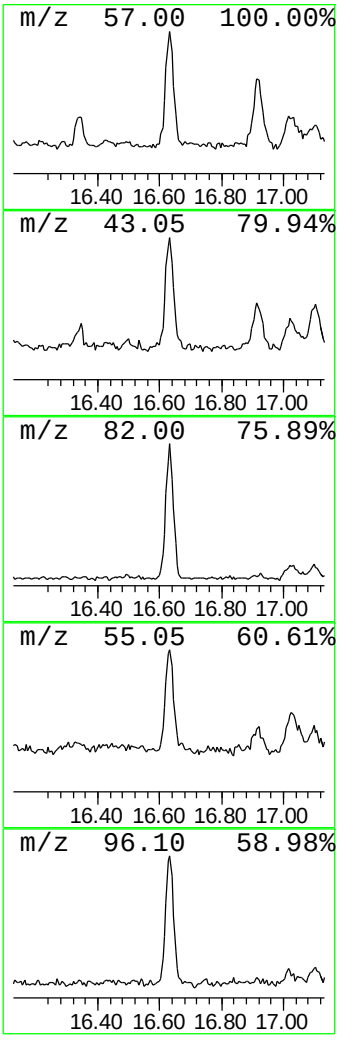
Peak Number 12 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	9.28 ng	354801	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
3	Octadecanal	268	C18H36O	000638-66-4	72
4	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	60
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	52





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Sample : I6908-07
Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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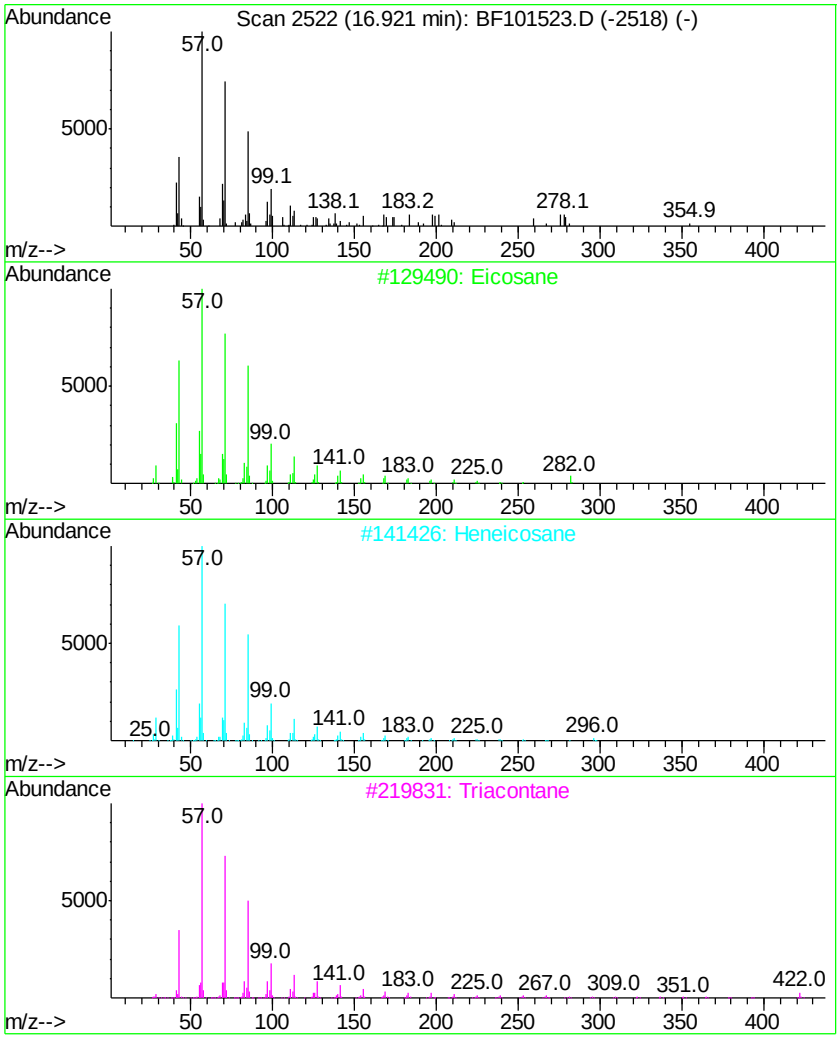
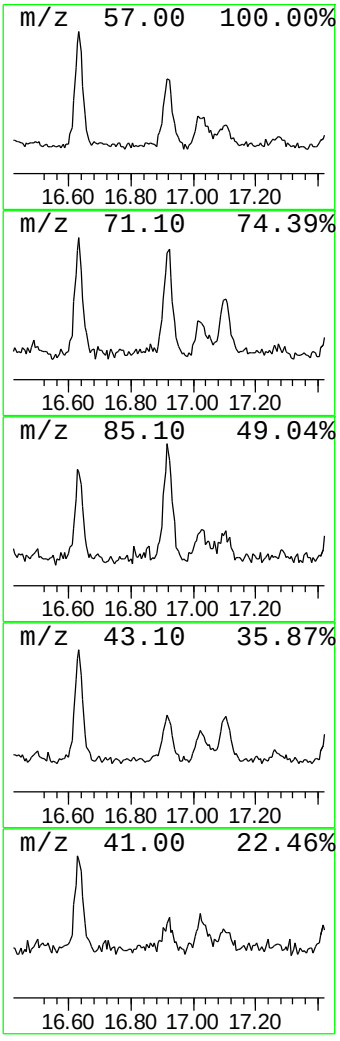
Peak Number 13 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.92	3.86 ng	147618	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	80
2	Heneicosane	296	C21H44	000629-94-7	80
3	Triacontane	422	C30H62	000638-68-6	80
4	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	72
5	Hentriacontane	437	C31H64	000630-04-6	64





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Sample : I6908-07
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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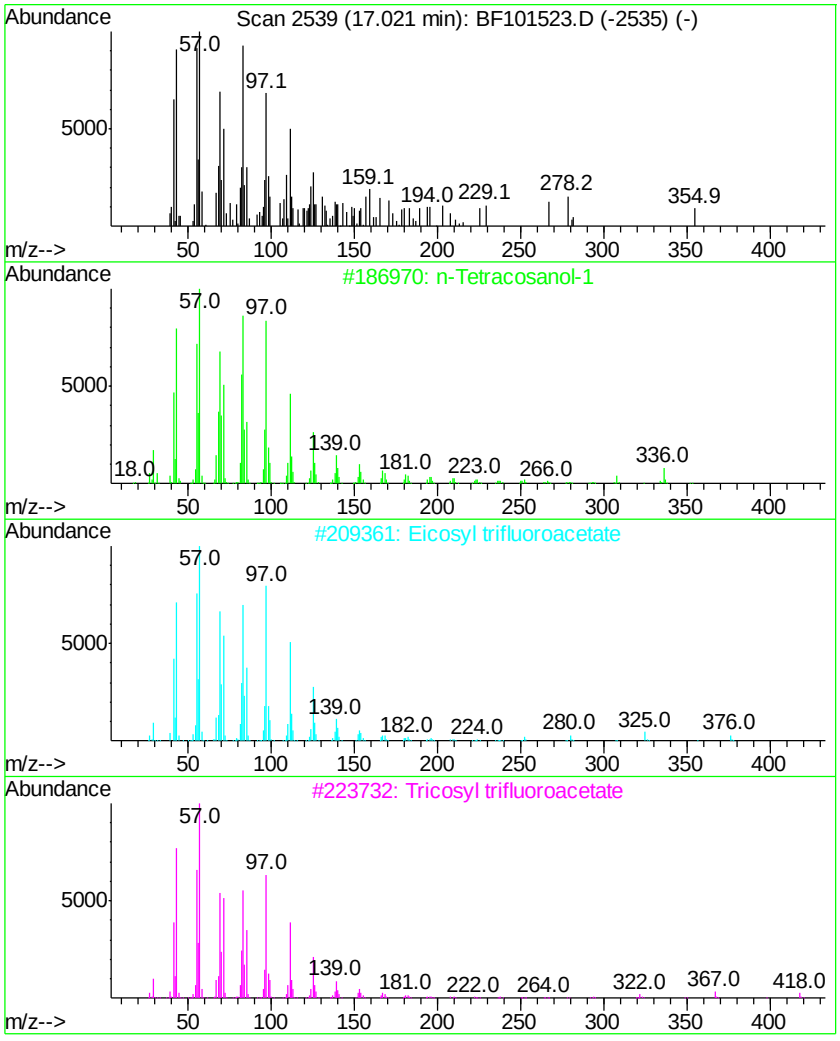
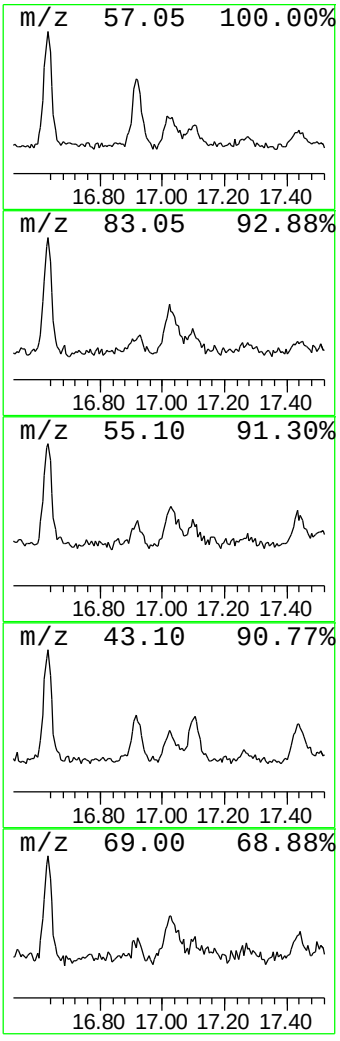
Peak Number 14 n-Tetracosanol-1 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	3.43 ng	131264	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	62
2	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	55
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	55
4	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	55
5	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	55





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Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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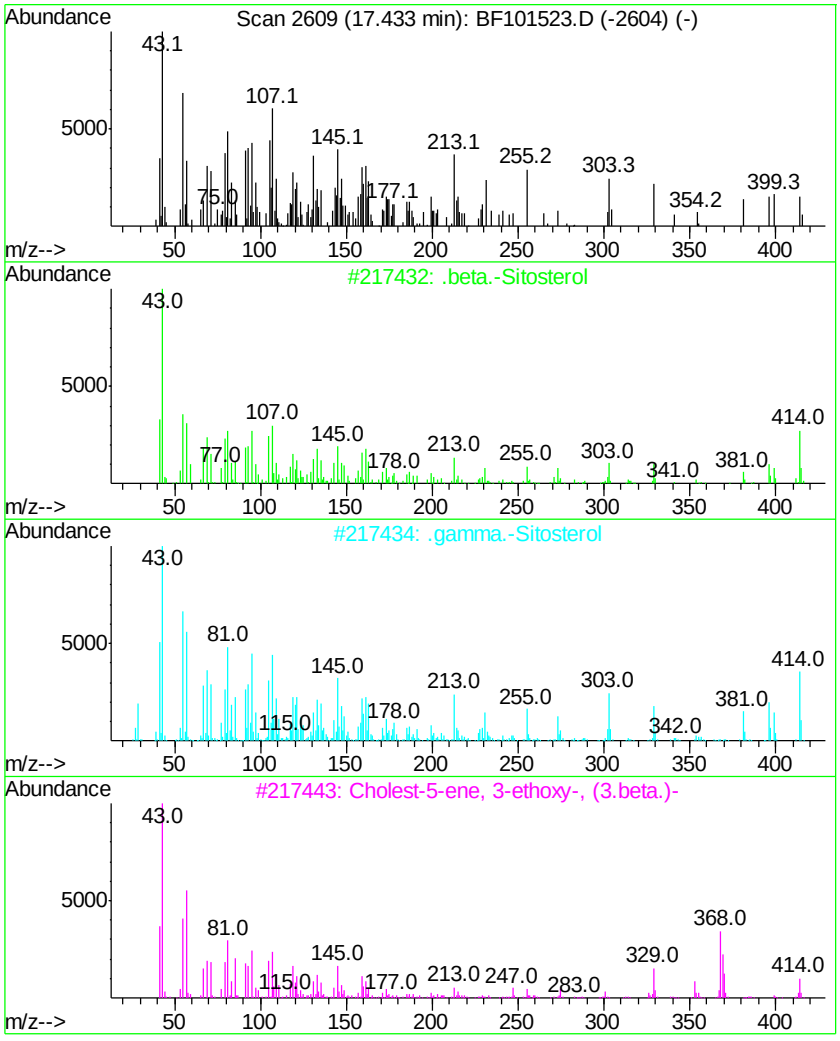
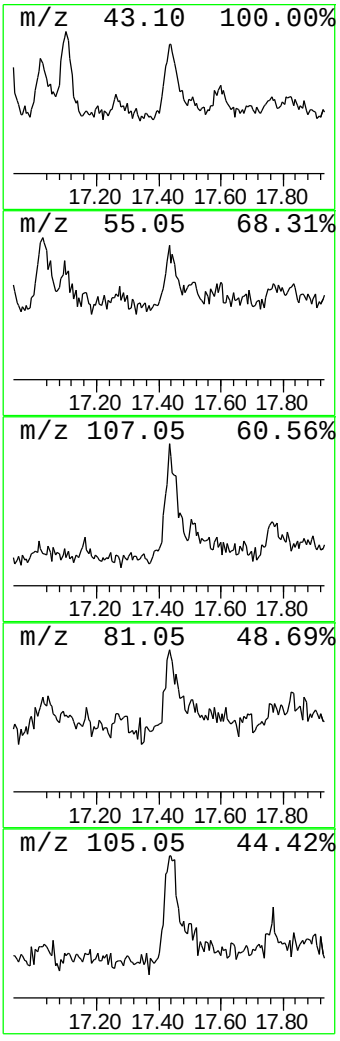
Peak Number 15 .beta.-Sitosterol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.43	5.64 ng	215632	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	91
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	87
3	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	46
4	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	42
5	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	27





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Operator : SJ/JU
Sample : I6908-07
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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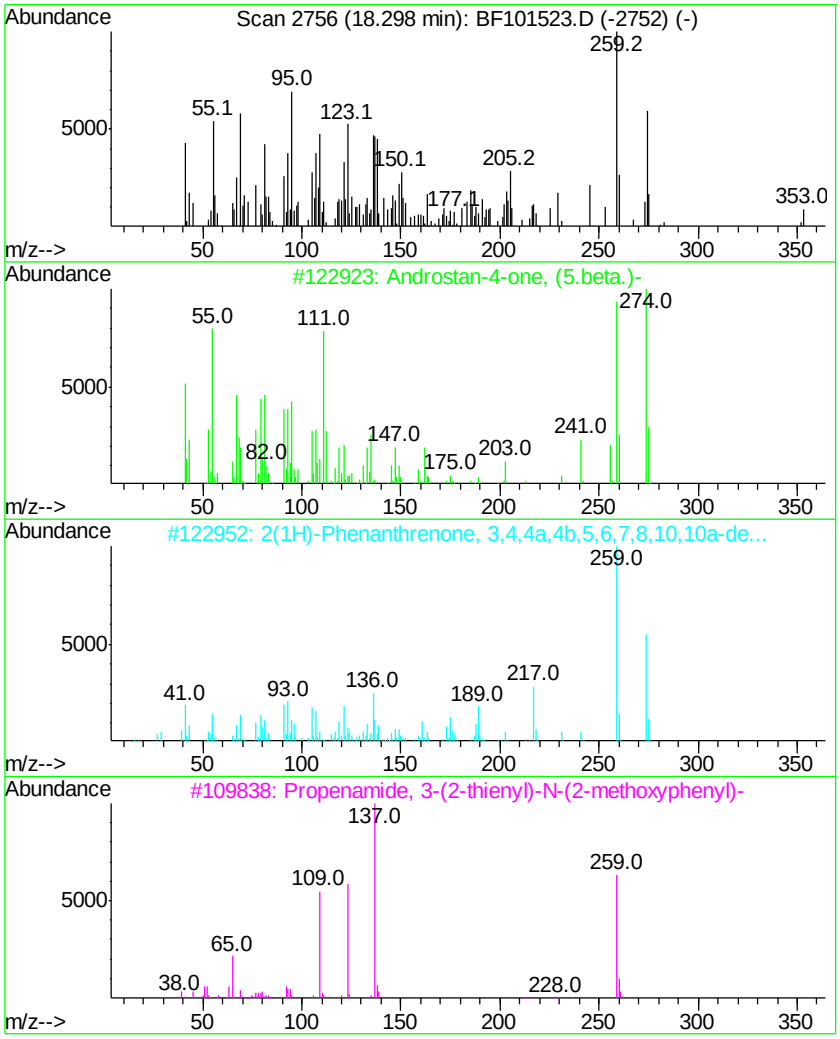
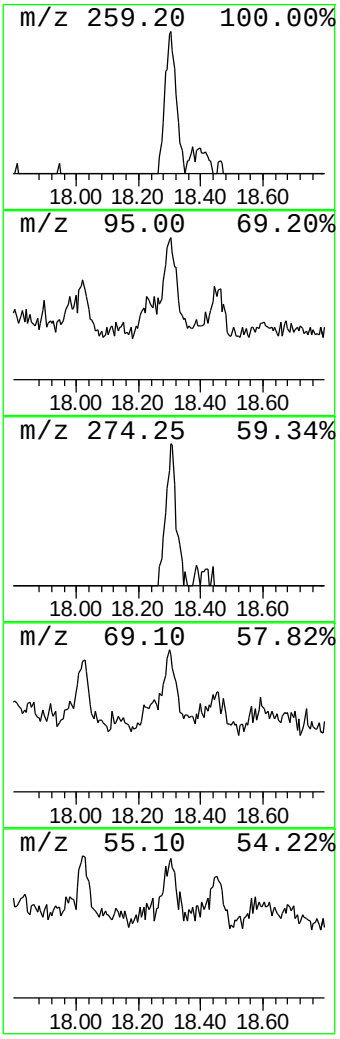
Peak Number 16 unknown18.30 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	6.61 ng	252845	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Androstan-4-one, (5.beta.)-	274	C19H30O	013583-71-6	43
2	2(1H)-Phenanthrenone, 3,4,4a,4b,...	274	C19H30O	007715-44-8	38
3	Propenamide, 3-(2-thienyl)-N-(2-...	259	C14H13NO2S	006906-11-2	35
4	1-(4-Undecylphenyl)ethanone	274	C19H30O	1000185-92-4	11
5	.delta.-3-1,2,5-Phosphasilaborol...	274	C15H24BPSi	1000152-86-1	11





Tentatively Identified Compound (LSC) summary

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Acq On : 19 Dec 2017 15:38
Operator : SJ/JU
Sample : I6908-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

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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...	5.03	16.6	ng	683631	1	6.81	823248	20.0
unknown6.58	6.58	65.7	ng	2703260	1	6.81	823248	20.0
1-Heneicosanol	13.80	13.3	ng	509318	5	13.99	768206	20.0
Heptadecyl heptaf...	14.44	8.3	ng	318916	5	13.99	768206	20.0
Hexacosane	15.06	17.5	ng	669115	6	15.46	764739	20.0
Behenic alcohol	15.09	3.4	ng	130512	6	15.46	764739	20.0
Oxirane, heptadecyl-	15.63	4.0	ng	152702	6	15.46	764739	20.0
Octacosane	15.85	14.7	ng	560065	6	15.46	764739	20.0
1-Tricosene	15.91	3.7	ng	143131	6	15.46	764739	20.0
Oxirane, hexadecyl-	16.63	9.3	ng	354801	6	15.46	764739	20.0
Eicosane	16.92	3.9	ng	147618	6	15.46	764739	20.0
n-Tetracosanol-1	17.02	3.4	ng	131264	6	15.46	764739	20.0
.beta.-Sitosterol	17.43	5.6	ng	215632	6	15.46	764739	20.0
unknown18.30	18.30	6.6	ng	252845	6	15.46	764739	20.0