LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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	5.195	482	486	494	rVB	176289	205338	9.11%	0.794%
2	5.607	553	556	563	rBV	2070854	2152752	95.47%	8.323%
3	6.213	654	659	663	rBV	26964	36258	1.61%	0.140%
4	6.607	722	726	734	rBV	2321059	2105064	93.35%	8.138%
5	6.742	745	749	753	rBV	2398979	2115701	93.82%	8.179%
6	6.966	783	787	790	rBV	840927	694761	30.81%	2.686%
7	7.119	809	813	817	rBV	1874217	1695617	75.19%	6.555%
8	7.525	877	882	885	rBV	1481625	1399567	62.07%	5.411%
9	8.248	1001	1005	1008	rBV	995815	831402	36.87%	3.214%
10	9.319	1181	1187	1194	rBV	2487718	2194252	97.31%	8.483%
11	9.713	1250	1254	1260	rBV	221330	189094	8.39%	0.731%
12	9.919	1285	1289	1294	rBV2	44661	48498	2.15%	0.187%
13	10.007	1298	1304	1315	rVB	976136	893328	39.62%	3.454%
14	10.419	1372	1374	1377	rVB2	54522	41249	1.83%	0.159%
15	10.642	1406	1412	1414	rVB2	21090	24873	1.10%	0.096%
16	10.795	1434	1438	1442	rBV	1245151	1167845	51.79%	4.515%
17	10.895	1452	1455	1461	rVB2	50278	65772	2.92%	0.254%
18	11.342	1529	1531	1534	rBV	41289	34633	1.54%	0.134%
19	11.495	1554	1557	1560	rBV	832151	757654	33.60%	2.929%
20	11.519	1560	1561	1567	rVB	142981	117279	5.20%	0.453%
21	11.695	1588	1591	1595	rBV5	16111	28296	1.25%	0.109%
22	12.001	1640	1643	1645	rBV	24658	23743	1.05%	0.092%
23	12.113	1658	1662	1664	rBV2	33383	34903	1.55%	0.135%
24	12.177	1670	1673	1676	rBV2	26401	28336	1.26%	0.110%
25	12.442	1713	1718	1720	rBV3	40669	43743	1.94%	0.169%
26	12.524	1729	1732	1734	rBV3	21454	24671	1.09%	0.095%
27	12.713	1761	1764	1767	rBV	355380	282383	12.52%	1.092%
28	12.748	1767	1770	1773	rVB	156633	125447	5.56%	0.485%
29	12.871	1788	1791	1792	rBV2	33749	27683	1.23%	0.107%
30	12.942	1797	1803	1809	rBV	309649	353959	15.70%	1.368%
31	12.989	1809	1811	1815	rBV2	17663	23728	1.05%	0.092%
32	13.083	1823	1827	1830	rBV	1949908	1704031	75.57%	6.588%
33	13.218	1847	1850	1852	rBV	48910	39134	1.74%	0.151%
34	13.271	1856	1859	1862	rVV2	51164	59342	2.63%	0.229%

LSC Area Percent Report

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Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.336	1868	1870	1873	rBV	32705	23793	1.06%	0.092%
36	13.448	1887	1889	1891	rBV	40518	29299	1.30%	0.113%
37	13.542	1903	1905	1909	rVB4	46199	44994	2.00%	0.174%
38	13.971	1975	1978	1983	rBV3	198474	220800	9.79%	0.854%
39	14.154	2004	2009	2012	rBV2	900903	945224	41.92%	3.654%
40	14.177	2012	2013	2021	rVB	170776	157553	6.99%	0.609%
41	14.324	2025	2038	2041	rBV6	696594	2254968	100.00%	8.718%
42	14.630	2086	2090	2096	rBV2	224020	355251	15.75%	1.373%
43	15.101	2168	2170	2176	rVB	102242	107953	4.79%	0.417%
44	15.248	2192	2195	2198	rBV	117704	173060	7.67%	0.669%
45	15.307	2201	2205	2209	rVB	391408	436906	19.38%	1.689%
46	15.636	2258	2261	2267	rVV	96050	117450	5.21%	0.454%
47	15.706	2268	2273	2282	rVB	487799	696597	30.89%	2.693%
48	15.930	2308	2311	2317	rVB2	111518	158566	7.03%	0.613%
49	16.177	2350	2353	2359	rVB	145213	199255	8.84%	0.770%
50	17.042	2496	2500	2506	rVB3	88685	156275	6.93%	0.604%
51	17.900	2640	2646	2656	rVB3	76759	218039	9.67%	0.843%

Sum of corrected areas: 25866319

LSC Report - Integrated Chromatogram

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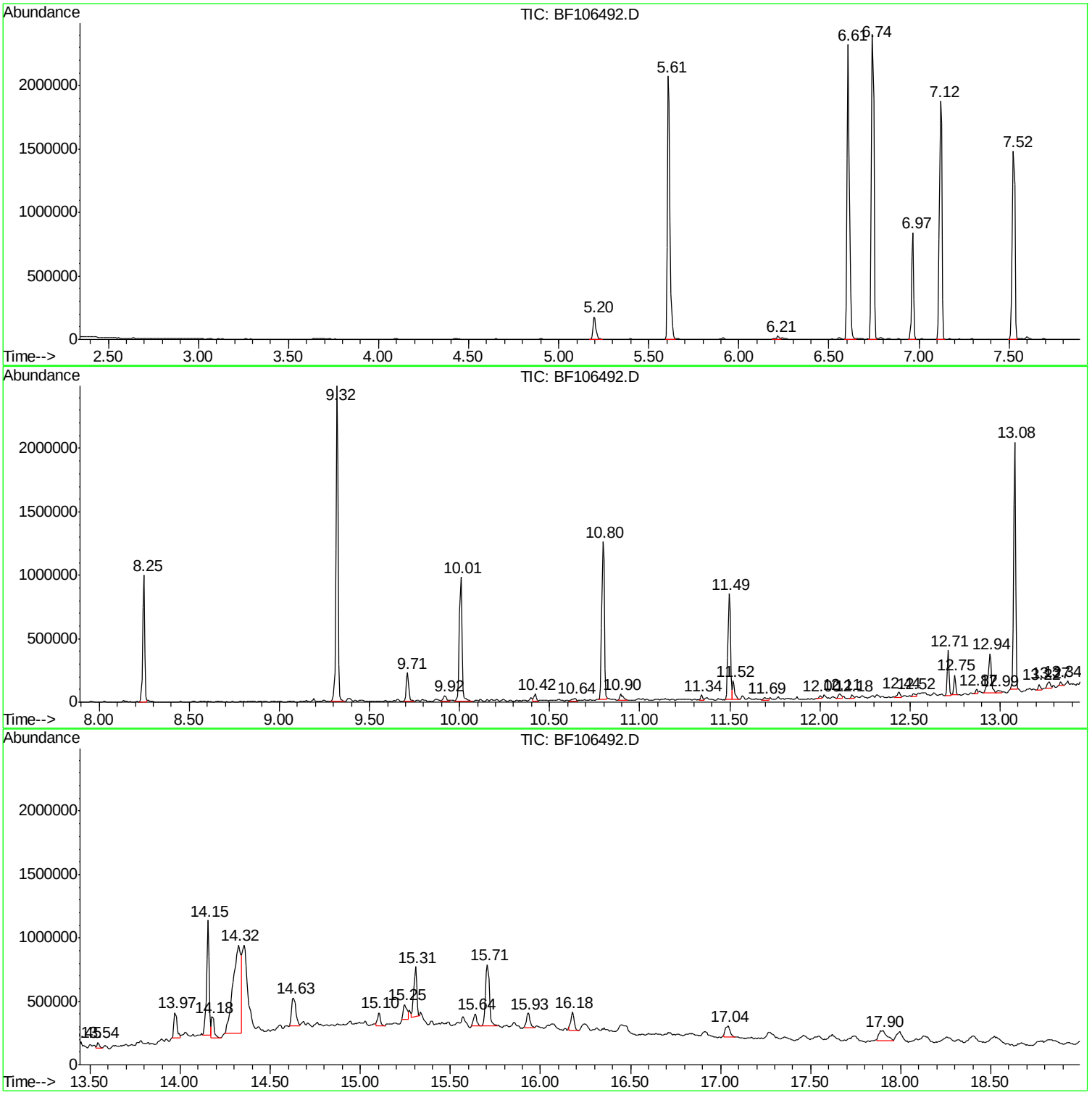
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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 : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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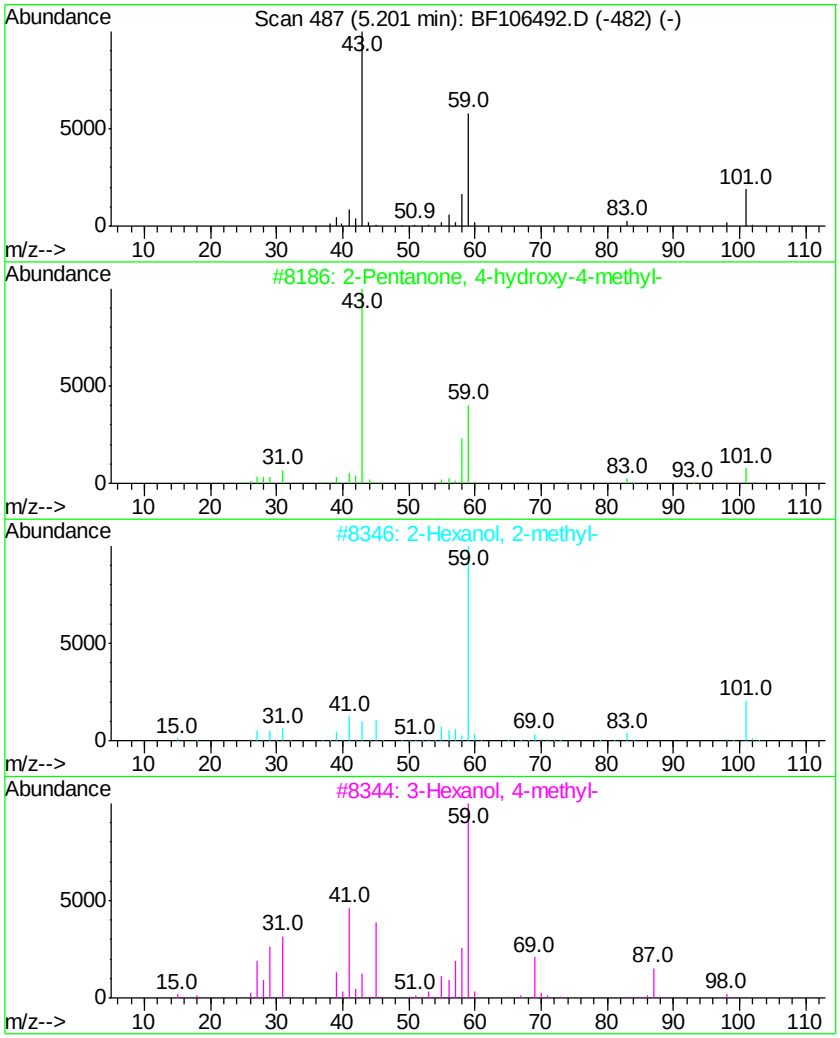
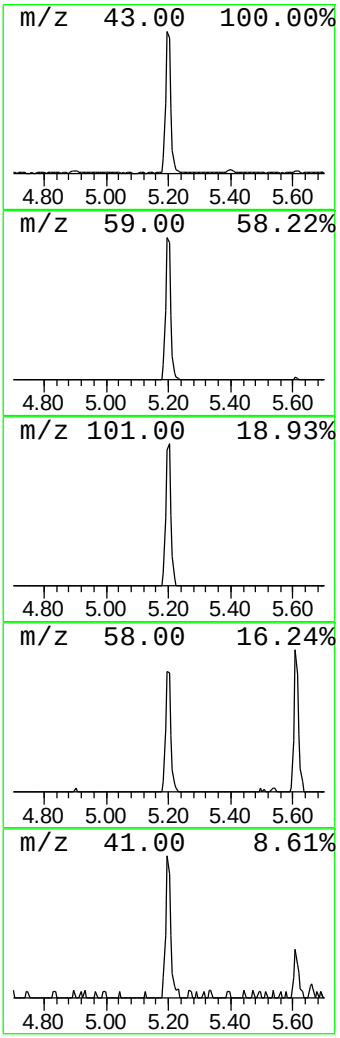
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.91 ng	205338	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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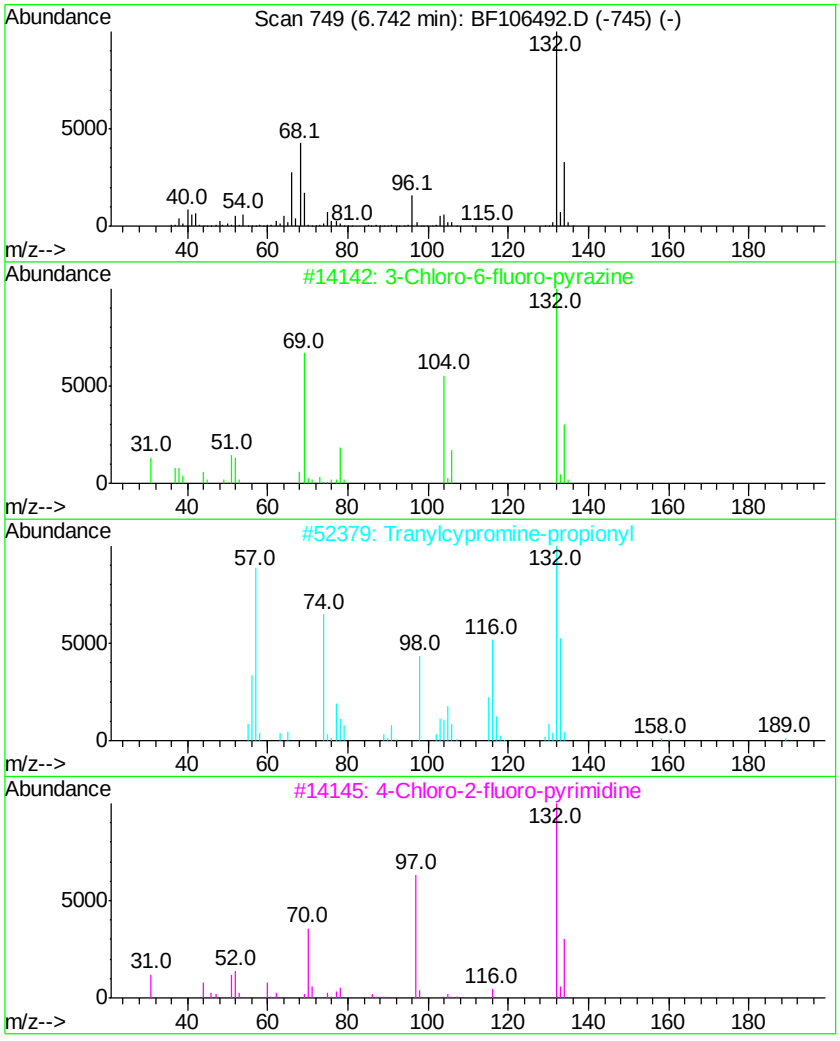
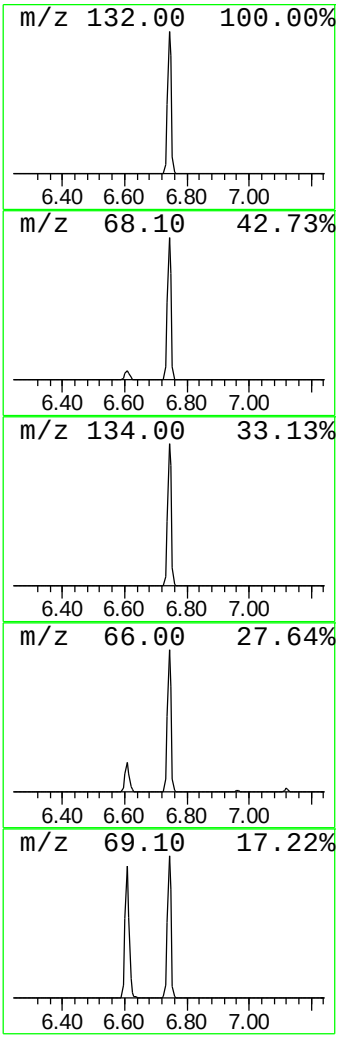
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	60.90 ng	2115700	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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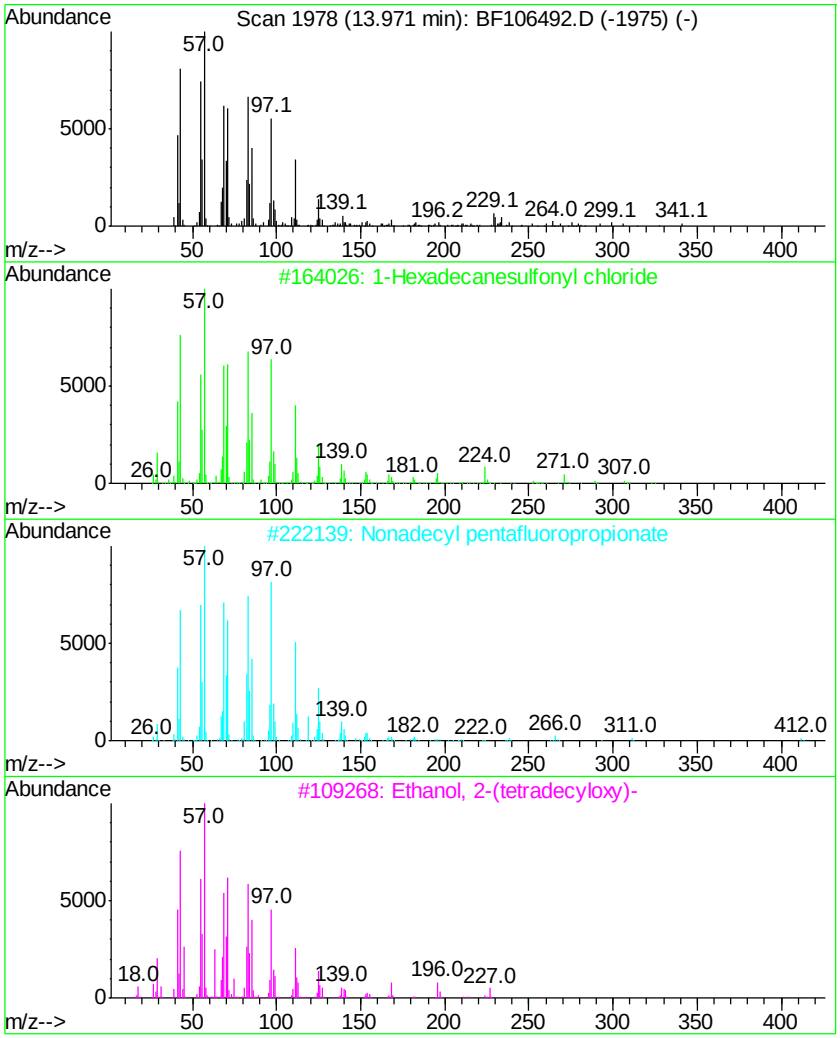
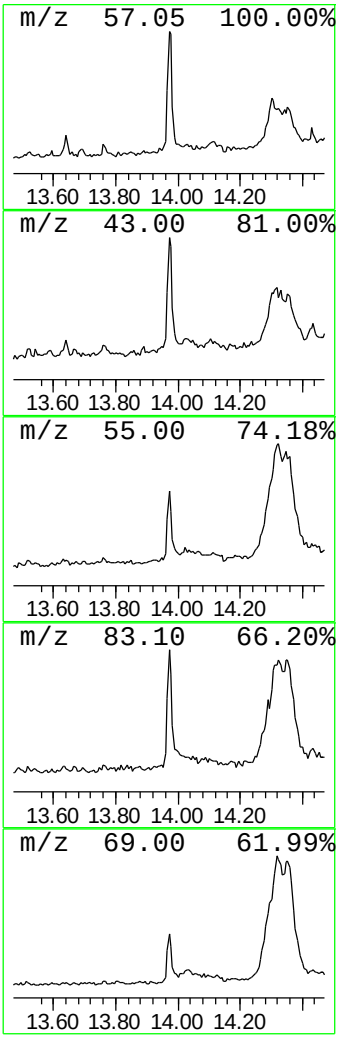
Peak Number 4 1-Hexadecanesulfonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.67 ng	220800	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

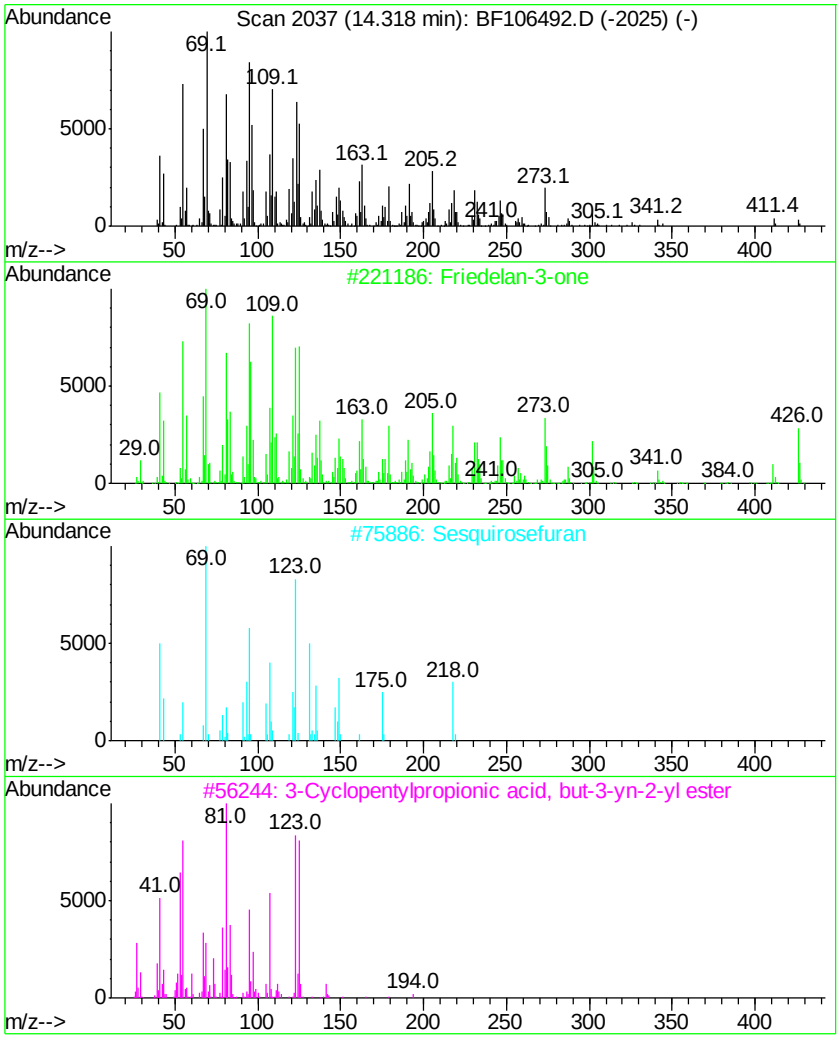
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

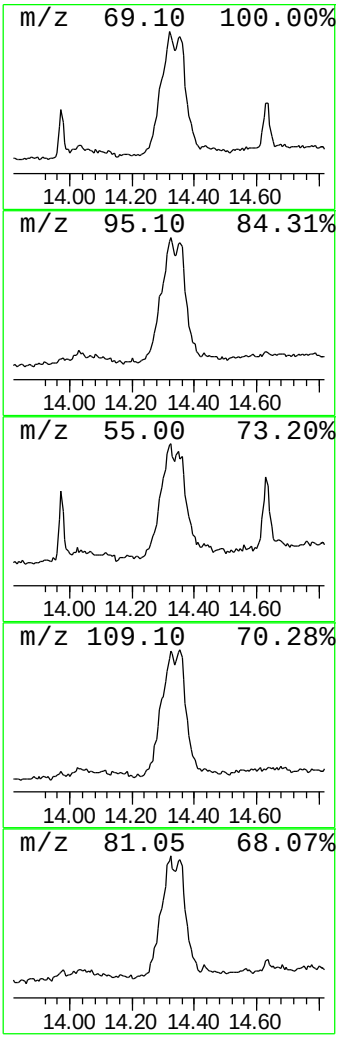
****

Peak Number 5 Friedelan-3-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	47.71 ng	2254970	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Friedelan-3-one	426	C30H50O	000559-74-0	89
2	Sesquirosefuran	218	C15H22O	039007-93-7	60
3	3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	60
4	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
5	D:A-Friedoursan-3-one	426	C30H50O	089950-00-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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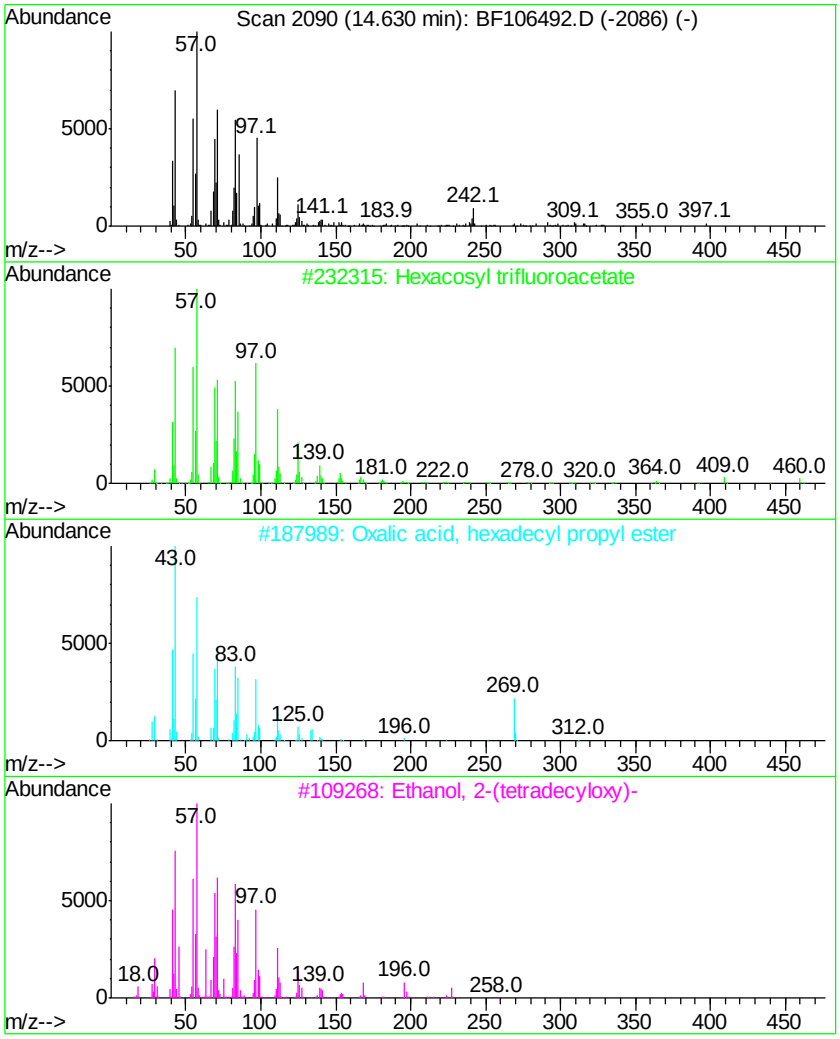
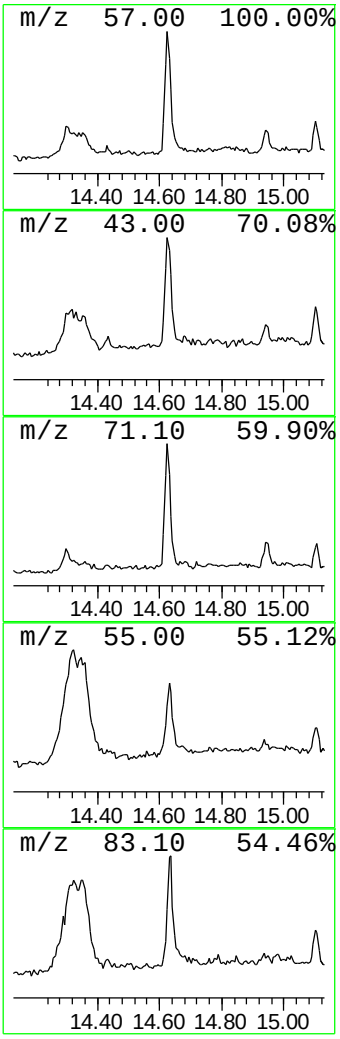
Peak Number 6 Hexacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	7.52 ng	355251	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
2	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
5	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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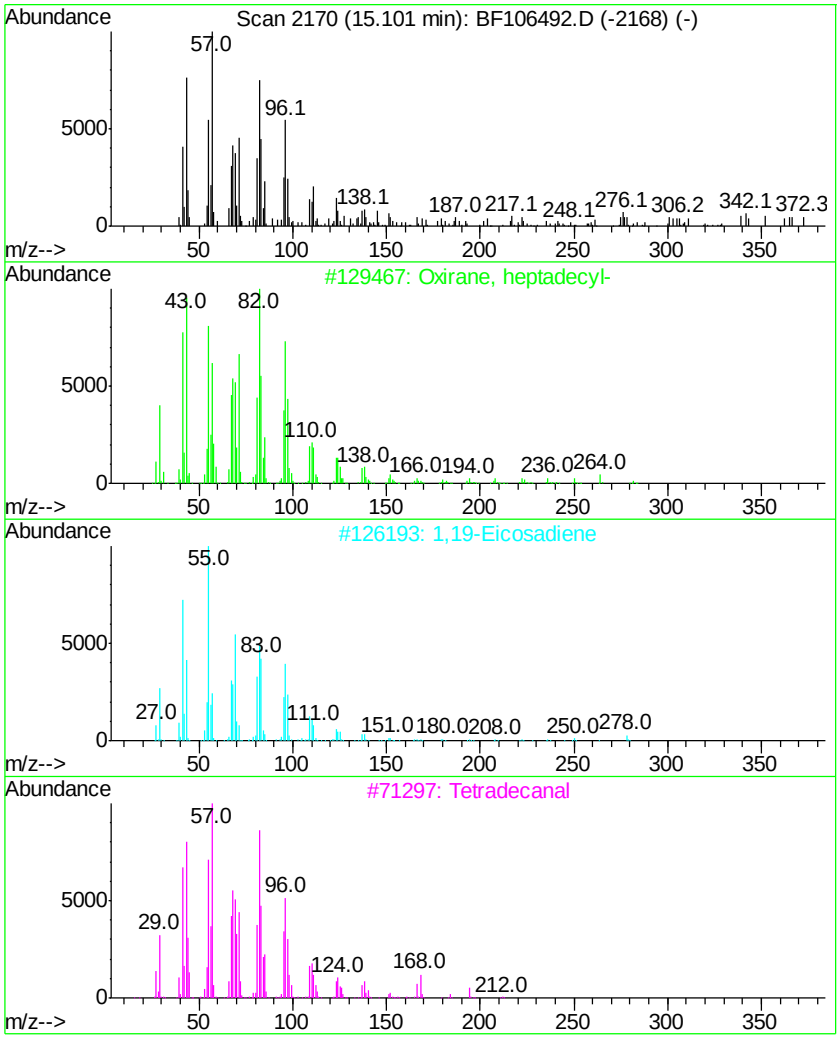
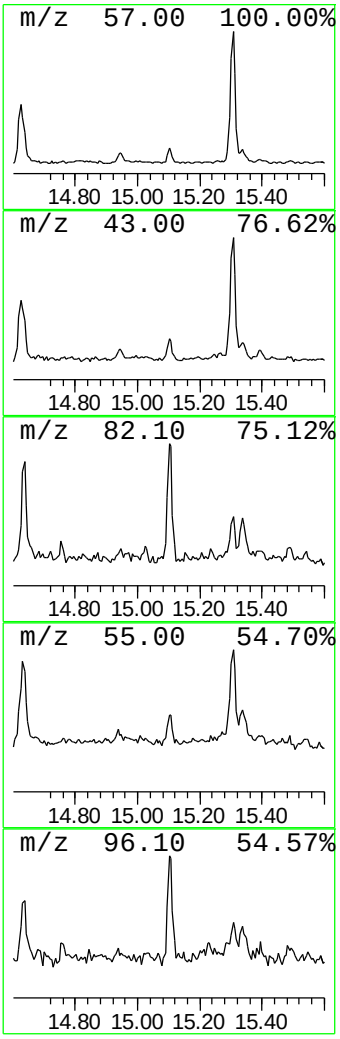
Peak Number 7 Oxirane, heptadecyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	3.10 ng	107953	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	1,19-Eicosadiene	278	C20H38	014811-95-1	90
3	Tetradecanal	212	C14H28O	000124-25-4	90
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
5	Tridecanal	198	C13H26O	010486-19-8	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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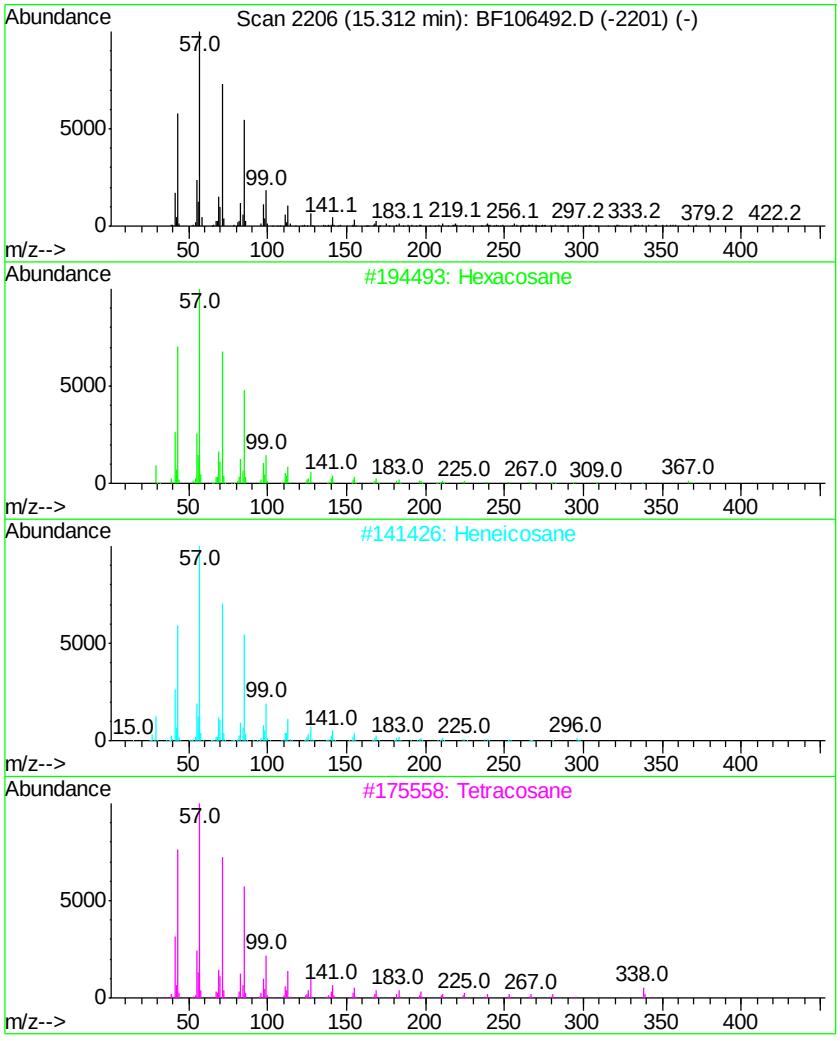
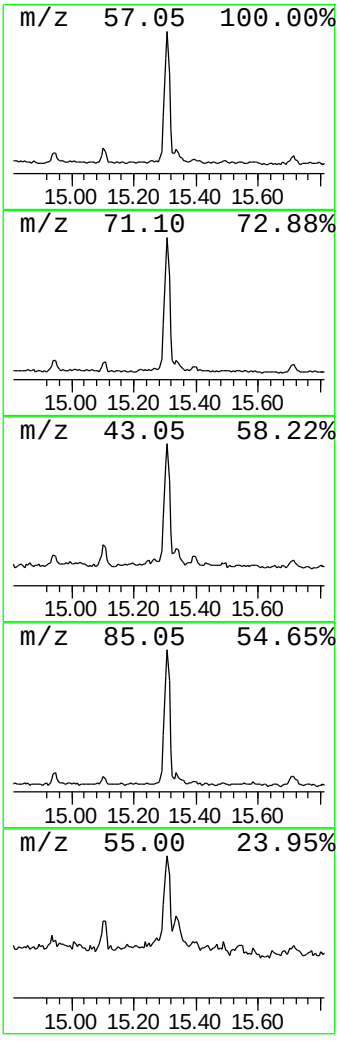
Peak Number 8 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	12.54 ng	436906	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Docosane	310	C22H46	000629-97-0	90
5	Triacontane	422	C30H62	000638-68-6	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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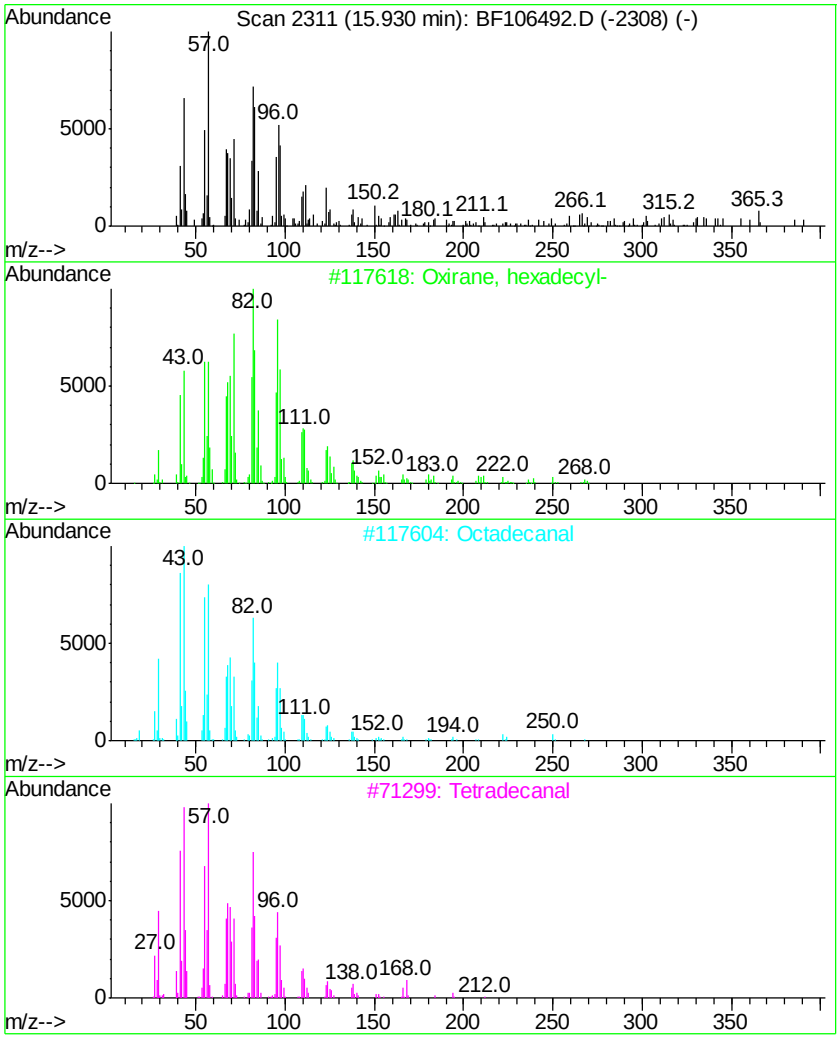
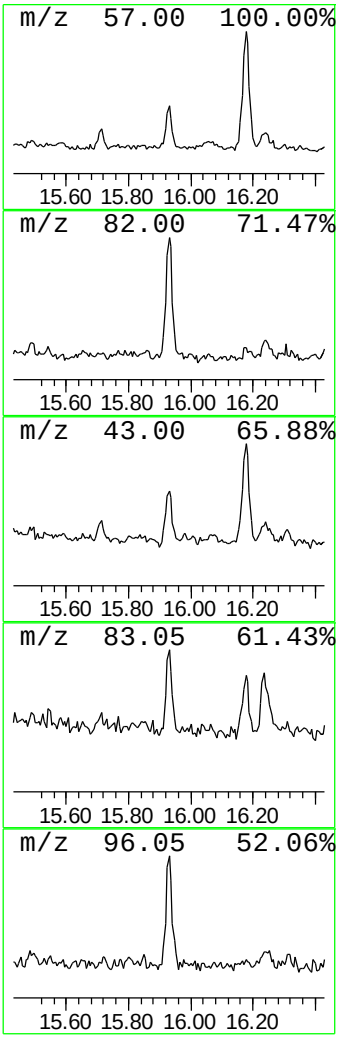
Peak Number 9 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.55 ng	158566	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2	Octadecanal	268	C18H36O	000638-66-4	86
3	Tetradecanal	212	C14H28O	000124-25-4	76
4	Tridecane, 1-bromo-	262	C13H27Br	000765-09-3	56
5	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	53





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Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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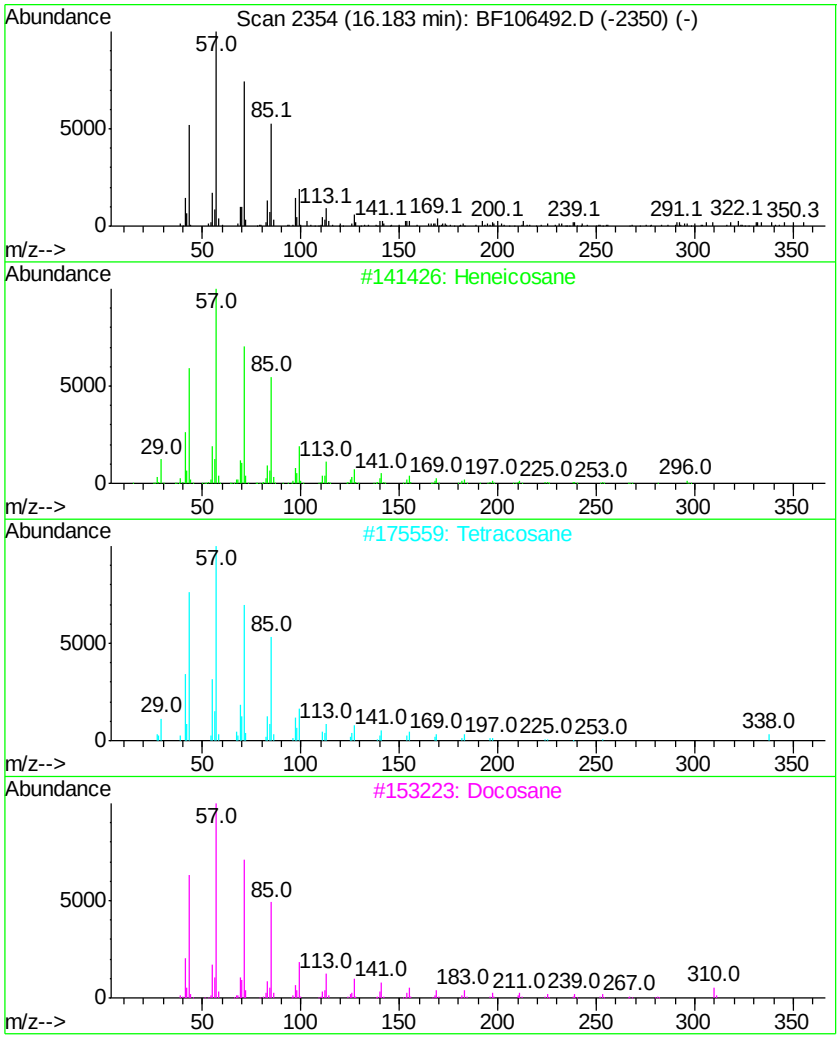
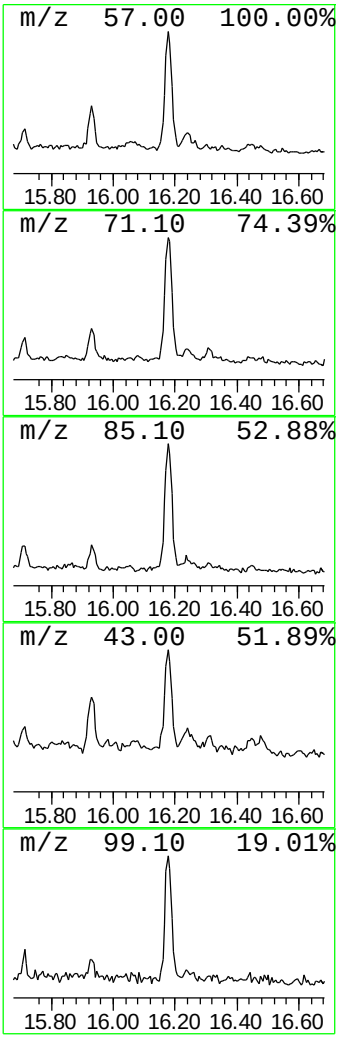
Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	5.72 ng	199255	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Tetracosane	338	C24H50	000646-31-1	93
3	Docosane	310	C22H46	000629-97-0	93
4	Pentacosane	352	C25H52	000629-99-2	93
5	Heptadecane	240	C17H36	000629-78-7	87





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Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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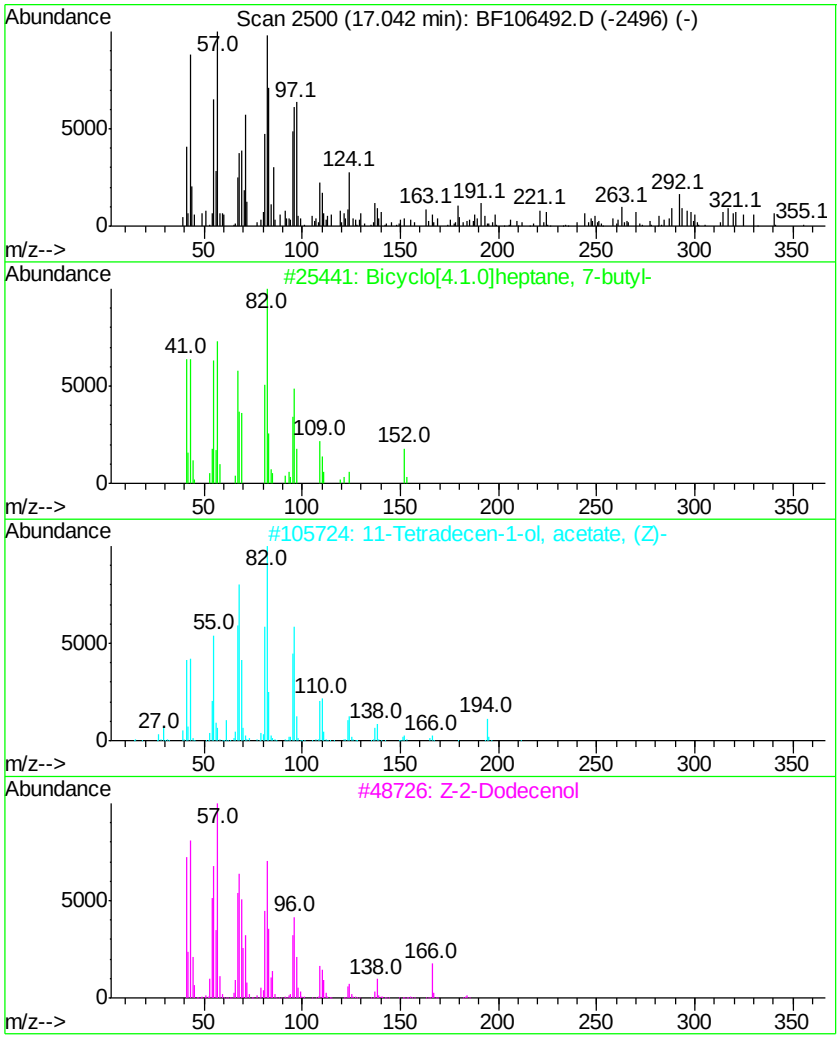
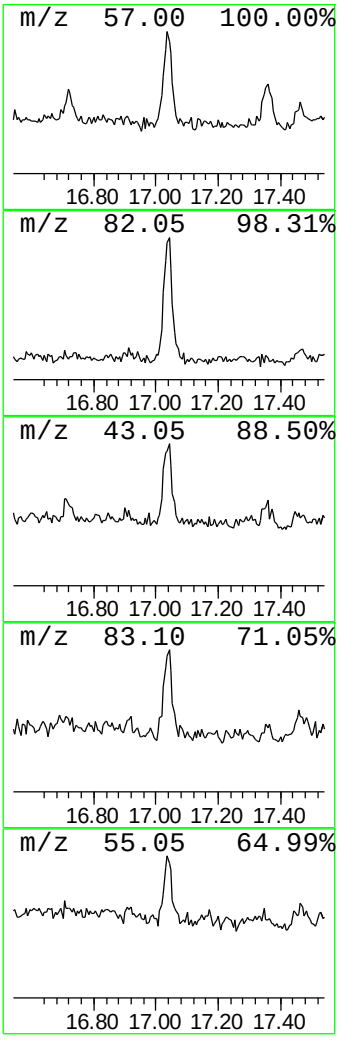
Peak Number 11 Bicyclo[4.1.0]heptane, 7-bu... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	4.49 ng	156275	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	64
2	11-Tetradecen-1-ol, acetate, (Z)-	254	C16H30O2	020711-10-8	50
3	Z-2-Dodecenol	184	C12H24O	069064-36-4	49
4	Methanamine, N-[3-methyl-2-buten...	97	C6H11N	1000196-86-4	43
5	E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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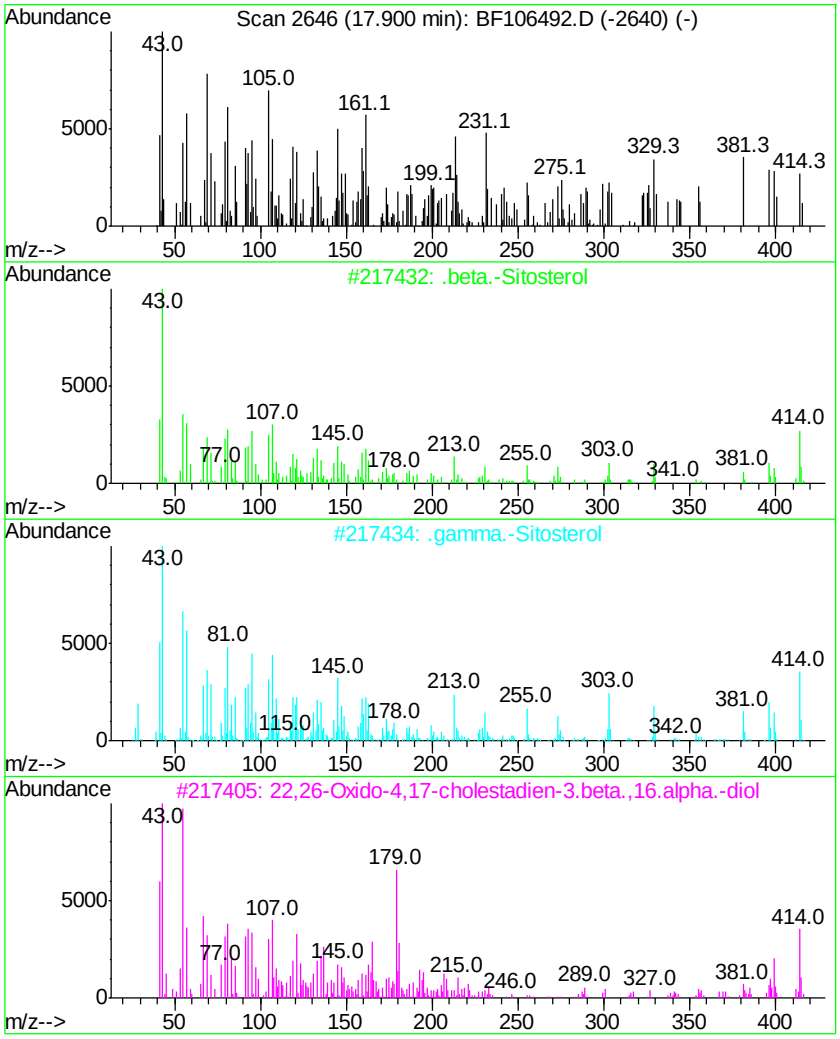
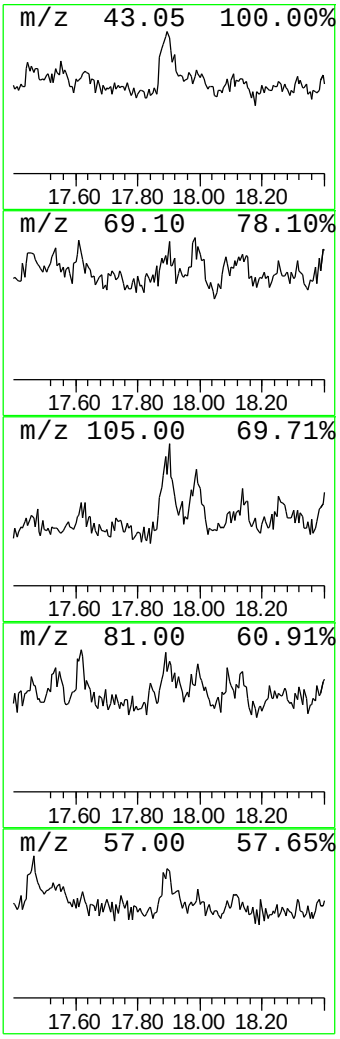
Peak Number 12 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	6.26 ng	218039	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	52
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	46
3	22,26-Oxido-4,17-cholestadien-3....	414	C27H42O3	1000252-80-4	10
4	Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H50O	006384-28-7	9
5	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061518\
Data File : BF106492.D
Acq On : 15 Jun 2018 15:28
Operator : JU/SJ
Sample : J3471-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : #2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.20	5.9	ng	205338	1	6.97	694761	20.0
unknown6.74	6.74	60.9	ng	2115700	1	6.97	694761	20.0
1-Hexadecanesulfo...	13.97	4.7	ng	220800	5	14.15	945224	20.0
Friedelan-3-one	14.32	47.7	ng	2254970	5	14.15	945224	20.0
Hexacosyl trifluo...	14.63	7.5	ng	355251	5	14.15	945224	20.0
Oxirane, heptadecyl-	15.10	3.1	ng	107953	6	15.71	696597	20.0
Hexacosane	15.31	12.5	ng	436906	6	15.71	696597	20.0
Oxirane, hexadecyl-	15.93	4.5	ng	158566	6	15.71	696597	20.0
Heneicosane	16.18	5.7	ng	199255	6	15.71	696597	20.0
Bicyclo[4.1.0]hep...	17.04	4.5	ng	156275	6	15.71	696597	20.0
.beta.-Sitosterol	17.90	6.3	ng	218039	6	15.71	696597	20.0