LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108508.D
Acq On : 27 Aug 2018 14:15
Operator : JU/SJ
Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

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-BF080818.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	5.248	491	495	504	rVB	94512	121179	3.65%	0.448%
2	5.631	555	560	563	rBV	2940134	2659518	80.01%	9.841%
3	6.625	724	729	732	rBV	2915312	2857005	85.95%	10.572%
4	6.772	749	754	757	rBV	3197950	2853731	85.85%	10.559%
5	7.001	789	793	796	rBV	893696	786643	23.66%	2.911%
6	7.154	815	819	823	rBV	2517683	2205474	66.35%	8.161%
7	7.560	883	888	891	rBV	1870727	1852026	55.71%	6.853%
8	8.283	1007	1011	1014	rBV	1146551	976761	29.38%	3.614%
9	9.354	1189	1193	1197	rBV	3565038	3324108	100.00%	12.300%
10	9.748	1256	1260	1272	rVB	274577	264132	7.95%	0.977%
11	10.042	1306	1310	1317	rBV2	1256531	1138949	34.26%	4.214%
12	10.836	1441	1445	1457	rBV	2142171	1963098	59.06%	7.264%
13	11.536	1560	1564	1568	rBV	1108979	1039470	31.27%	3.846%
14	12.760	1766	1772	1775	rBV	37755	35395	1.06%	0.131%
15	12.989	1805	1811	1816	rBV	42877	55384	1.67%	0.205%
16	13.124	1830	1834	1837	rBV	2841037	2373322	71.40%	8.782%
17	14.036	1985	1989	1999	rBV3	78590	191981	5.78%	0.710%
18	14.189	2011	2015	2019	rBV	856994	824395	24.80%	3.050%
19	14.624	2086	2089	2094	rVB2	54310	60569	1.82%	0.224%
20	14.942	2139	2143	2150	rVB2	108925	162020	4.87%	0.600%
21	15.036	2155	2159	2164	rVB	125420	132919	4.00%	0.492%
22	15.283	2197	2201	2203	rBV	22670	36968	1.11%	0.137%
23	15.312	2203	2206	2211	rVB2	74449	89065	2.68%	0.330%
24	15.748	2272	2280	2287	rBV	560007	840811	25.29%	3.111%
25	16.195	2352	2356	2363	rVB	62145	101696	3.06%	0.376%
26	16.742	2445	2449	2455	rBV2	37469	78800	2.37%	0.292%

Sum of corrected areas: 27025419

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
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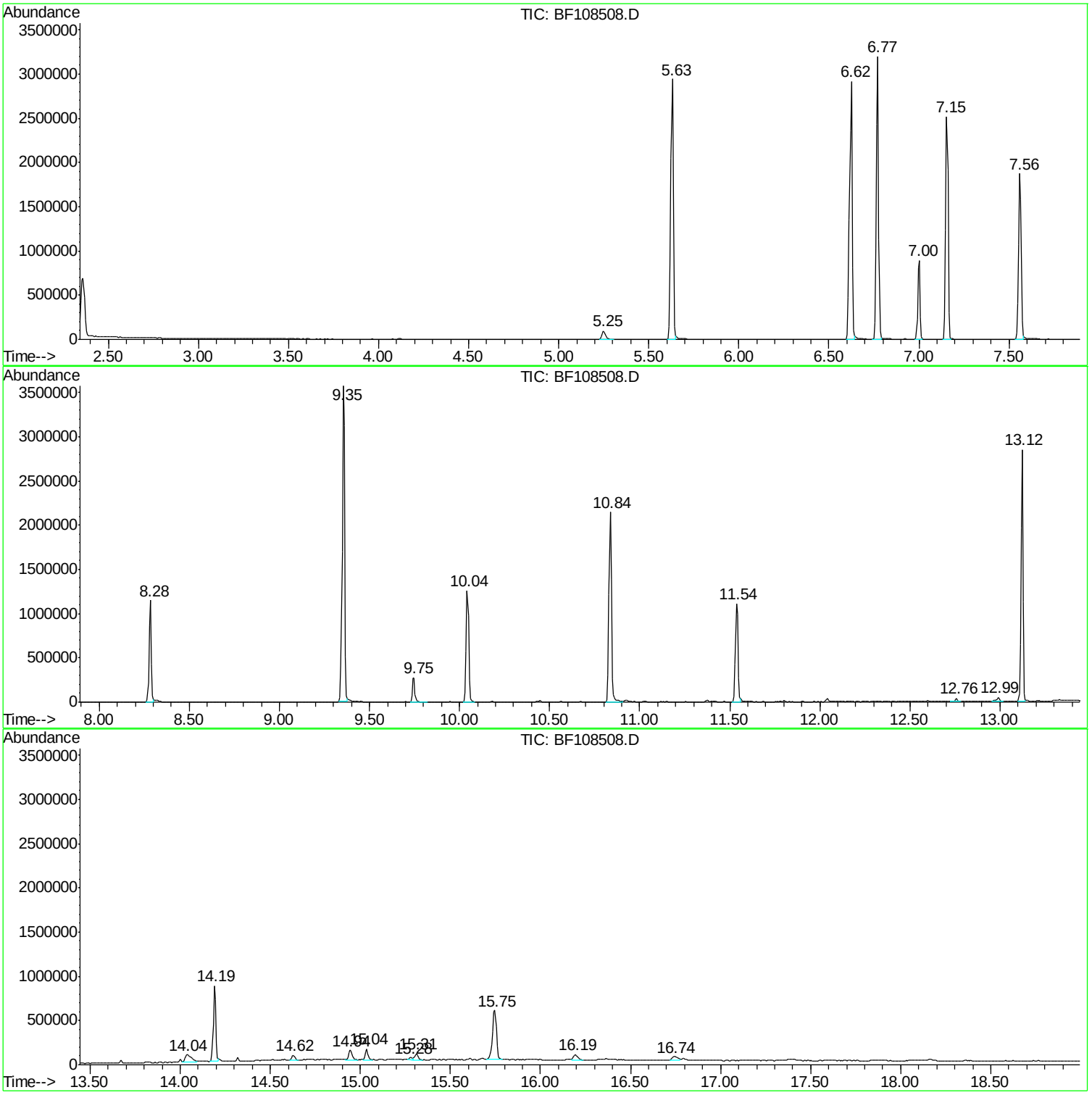
Operator : JU/SJ
Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF082718\
Data File : BF108508.D
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Operator : JU/SJ
Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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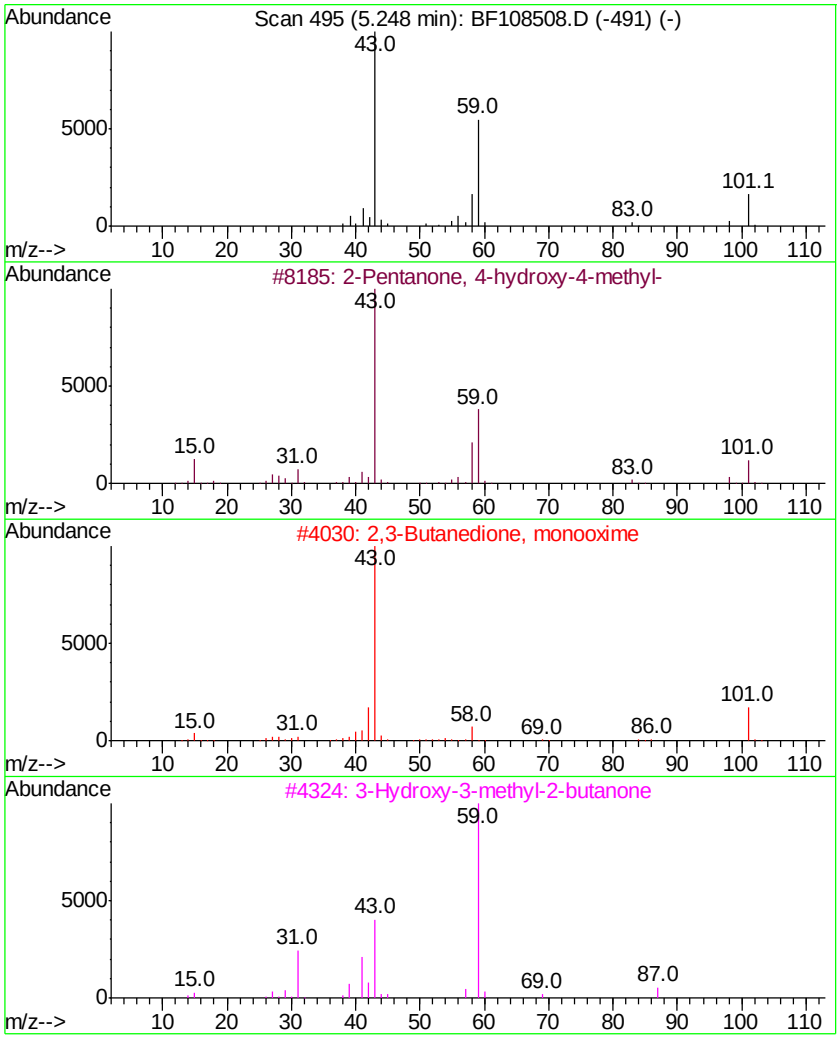
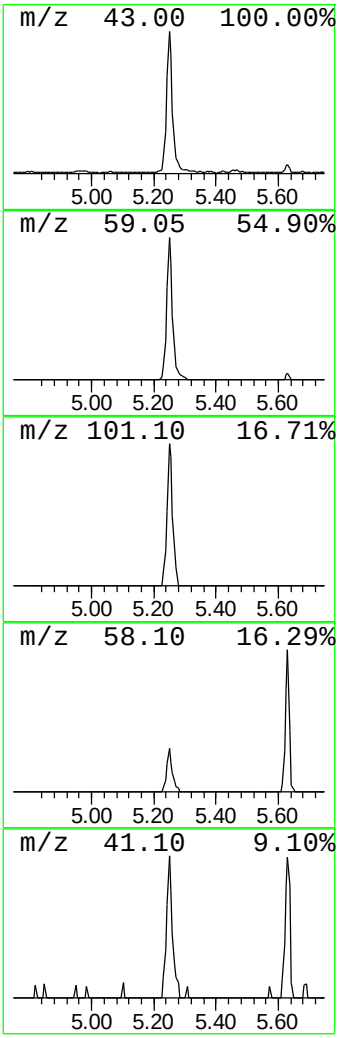
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	3.08 ng	121179	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





Library Search Compound Report

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Data File : BF108508.D
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Operator : JU/SJ
Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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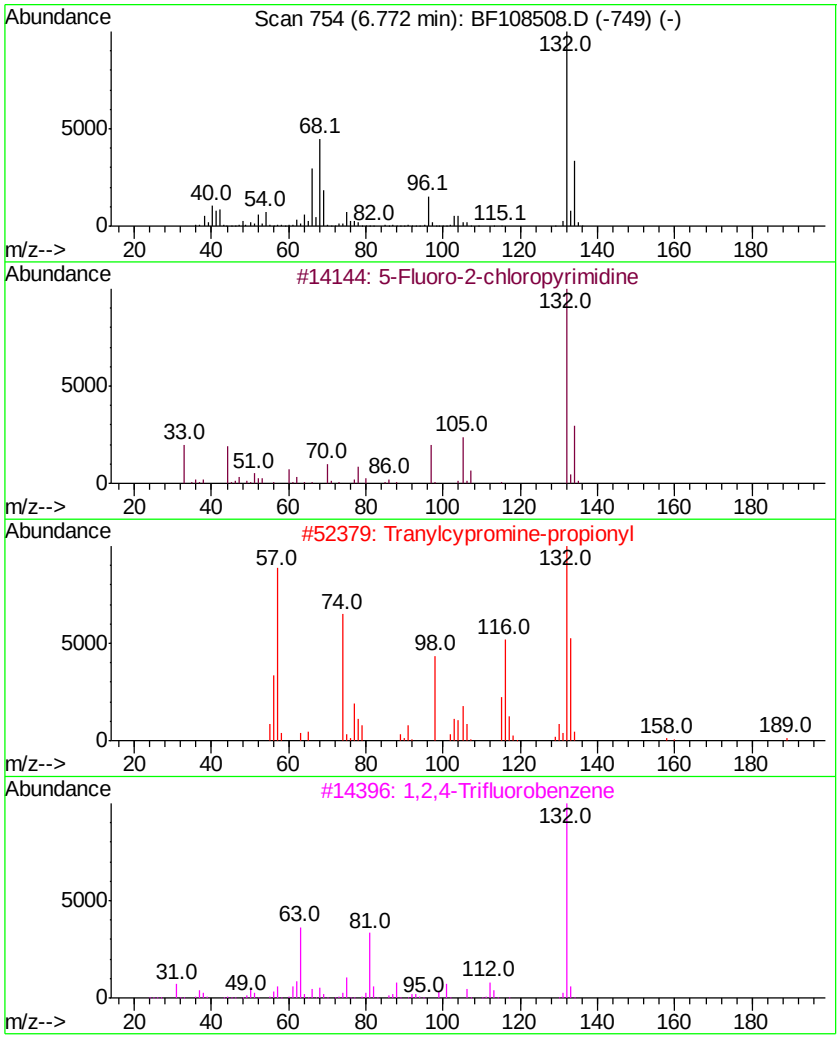
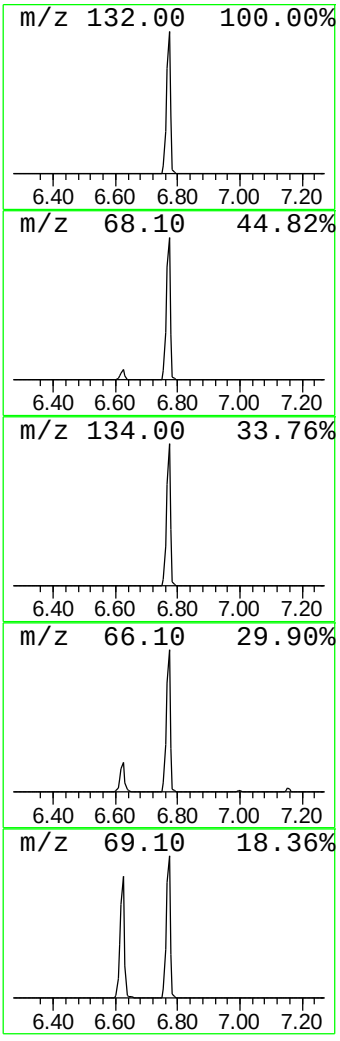
Peak Number 2 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	72.55 ng	2853730	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BF108508.D
Acq On : 27 Aug 2018 14:15
Operator : JU/SJ
Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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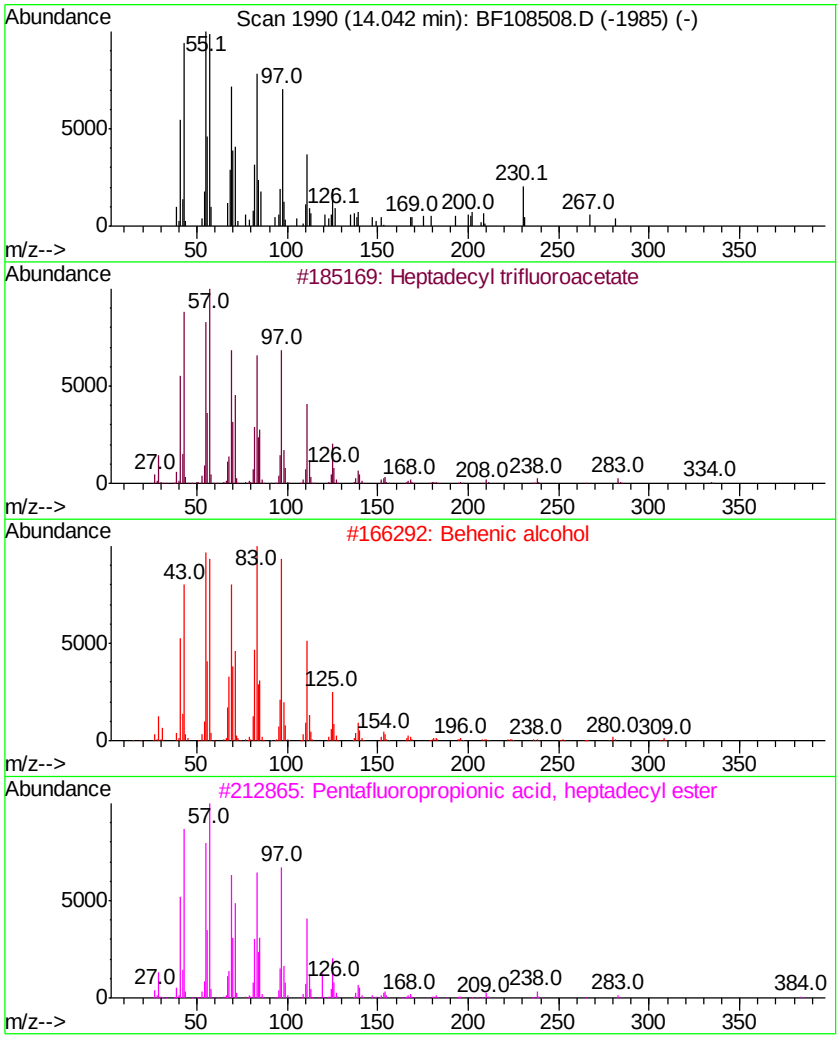
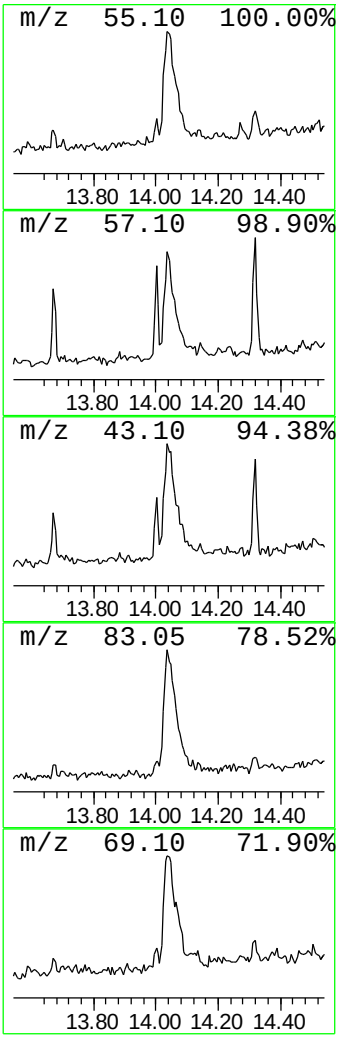
Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	4.66 ng	191981	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
2	Behenic alcohol	326	C22H46O	000661-19-8	87
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	86
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	83
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108508.D
Acq On : 27 Aug 2018 14:15
Operator : JU/SJ
Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

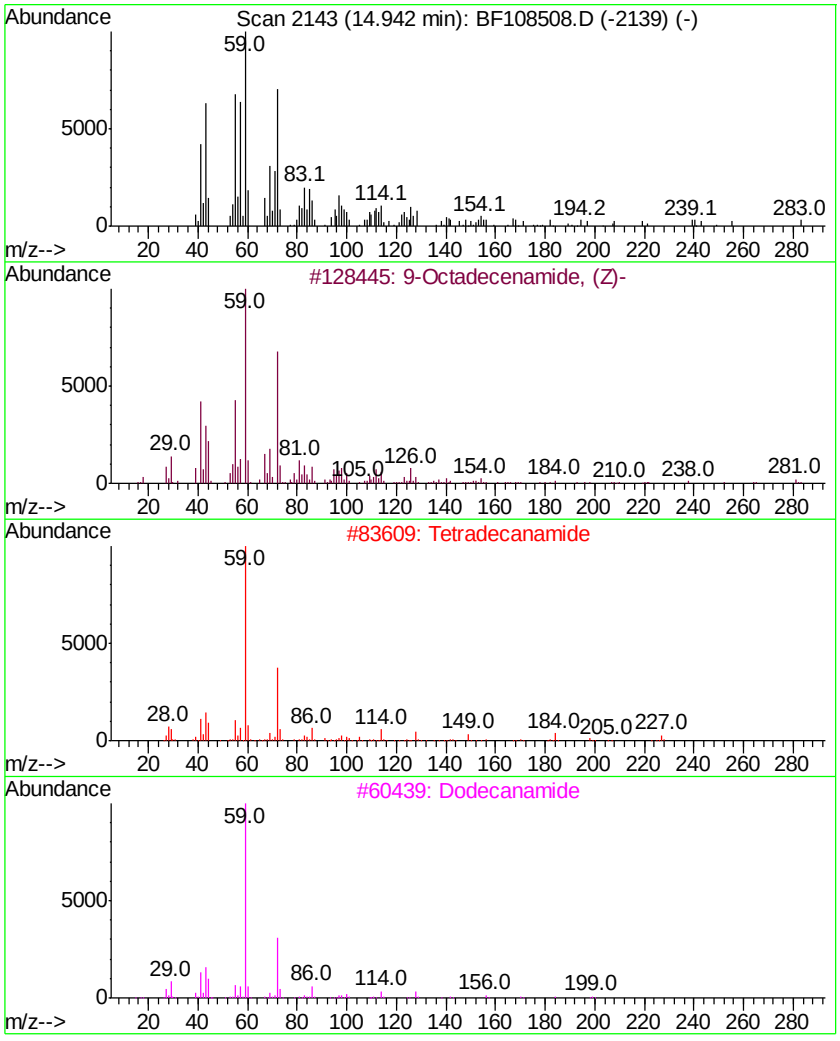
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

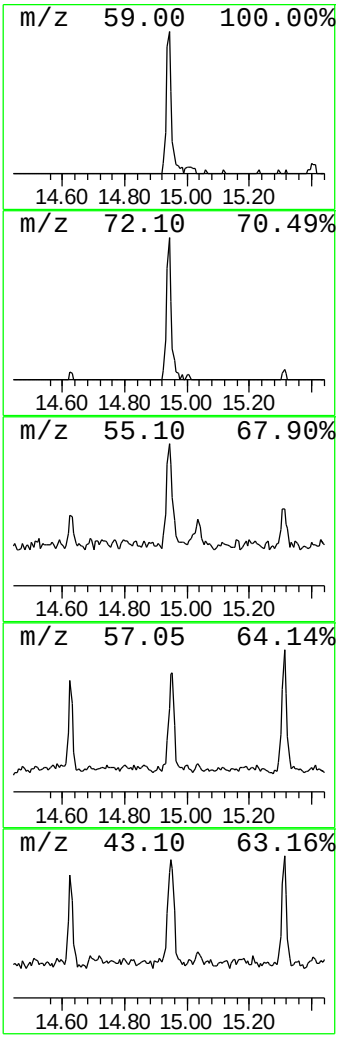
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	3.93 ng	162020	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	Dodecanamide	199	C12H25NO	001120-16-7	50
4	Octadecanamide	283	C18H37NO	000124-26-5	27
5	1-Heptadecanamine	255	C17H37N	004200-95-7	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
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Acq On : 27 Aug 2018 14:15
Operator : JU/SJ
Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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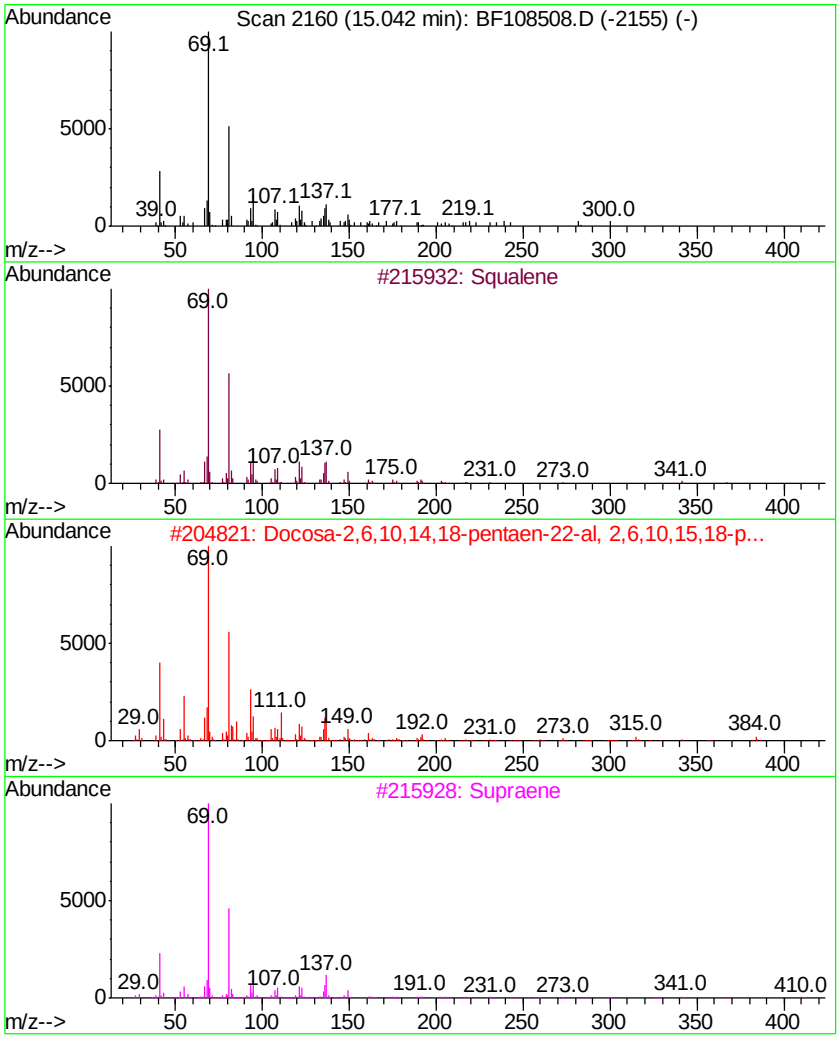
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

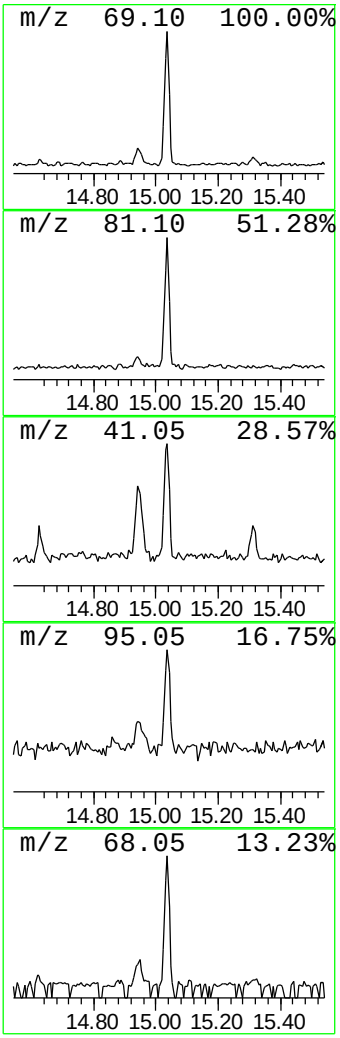
****

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	3.16 ng	132919	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3	Supraene	410	C30H50	007683-64-9	83
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	64





Library Search Compound Report

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Sample : J4646-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

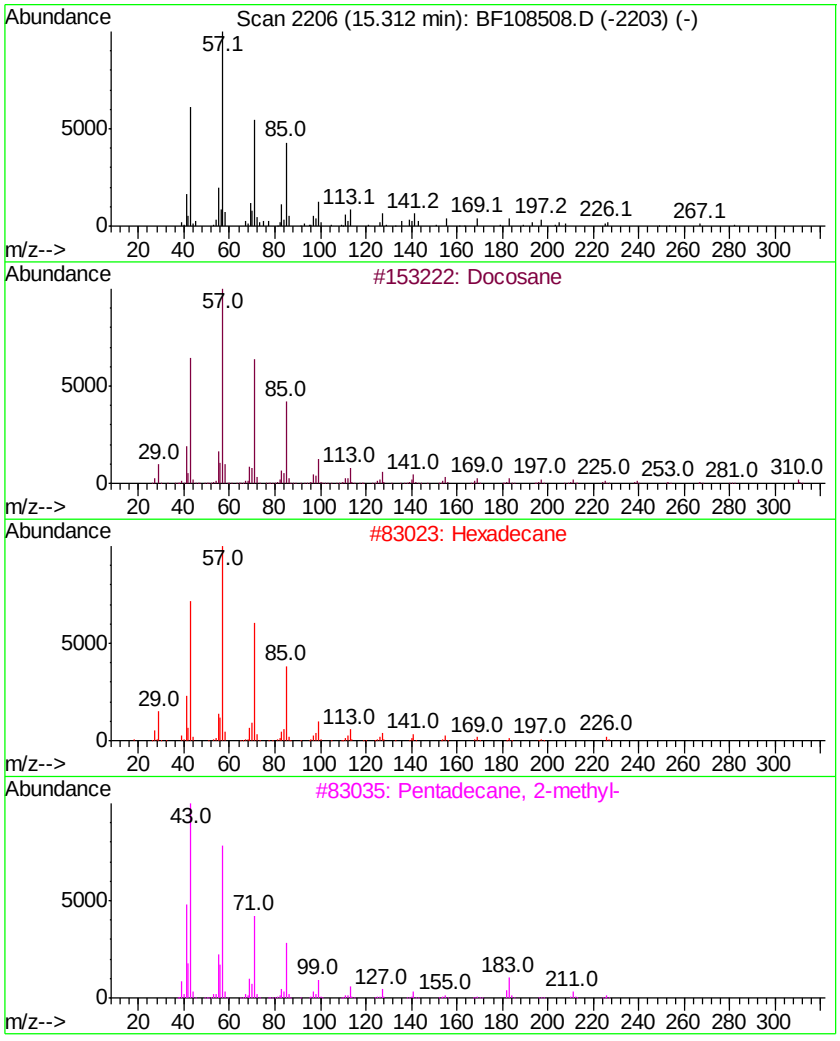
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

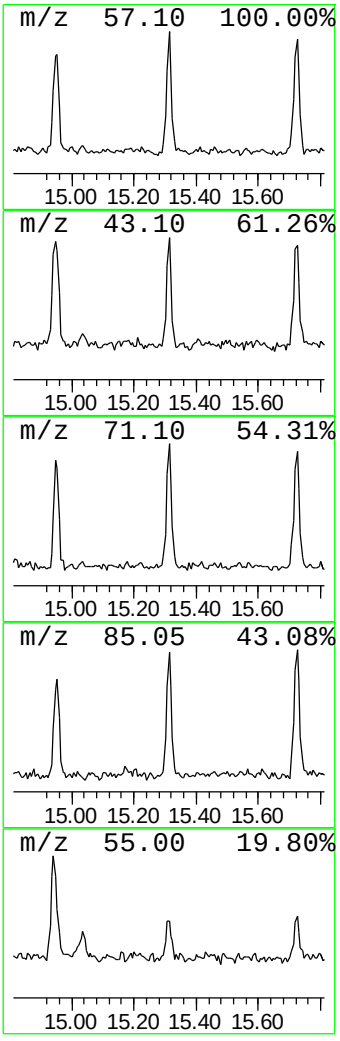
****

Peak Number 7 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.12 ng	89065	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	87
4	Triacontane	422	C30H62	000638-68-6	83
5	Hexacosane	366	C26H54	000630-01-3	81





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Instrument : BNA_F
ClientSampleId : EP1-Q4-B7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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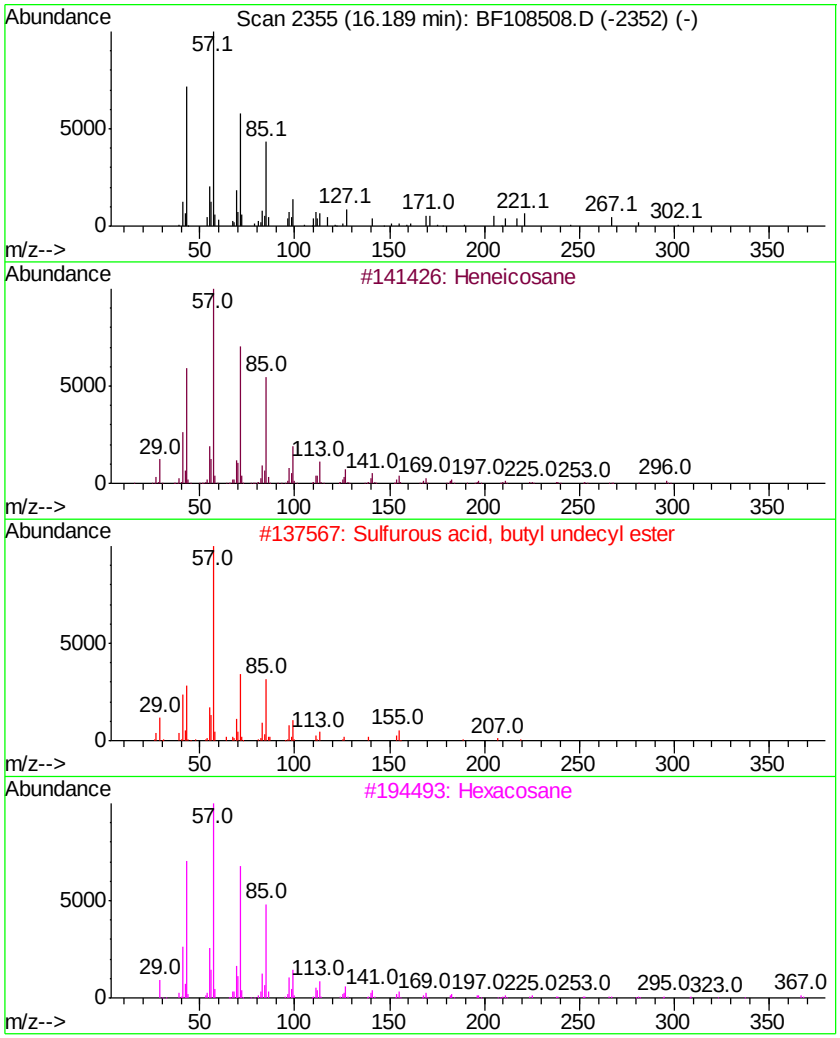
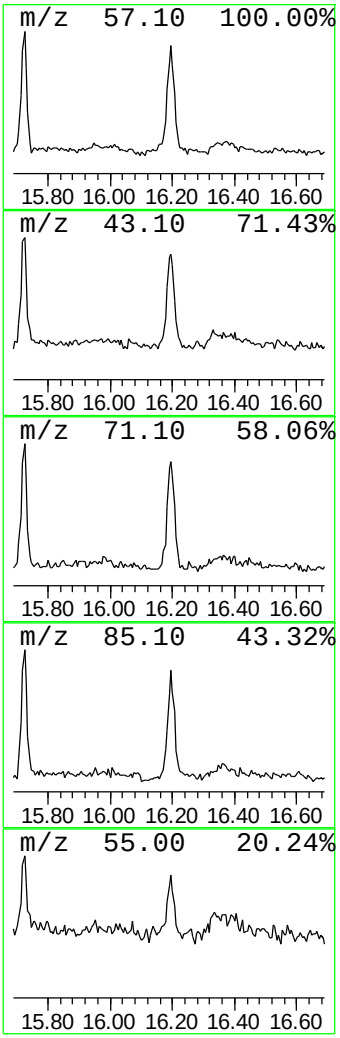
Peak Number 8 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.42 ng	101696	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	64
2	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	58
3	Hexacosane	366	C26H54	000630-01-3	52
4	Tetratetracontane	619	C44H90	007098-22-8	52
5	Tetracosane	338	C24H50	000646-31-1	52





Tentatively Identified Compound (LSC) summary

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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...	5.25	3.1	ng	121179	1	7.00	786643	20.0
unknown6.77	6.77	72.5	ng	2853730	1	7.00	786643	20.0
Heptadecyl triflu...	14.04	4.7	ng	191981	5	14.19	824395	20.0
9-Octadecenamide,...	14.94	3.9	ng	162020	5	14.19	824395	20.0
Squalene	15.04	3.2	ng	132919	6	15.75	840811	20.0
Docosane	15.31	2.1	ng	89065	6	15.75	840811	20.0
Heneicosane	16.19	2.4	ng	101696	6	15.75	840811	20.0