LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096911.D
Acq On : 20 Jul 2017 17:47
Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-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-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	4.746	464	469	486	rVB	207803	343508	9.96%	1.292%
2	5.181	537	543	546	rBV	2691785	2971631	86.20%	11.174%
3	6.228	714	721	735	rBV	2721820	3447329	100.00%	12.963%
4	6.340	735	740	743	rBV	2955916	3182862	92.33%	11.968%
5	6.569	775	779	783	rBV	723715	643632	18.67%	2.420%
6	6.728	801	806	809	rBV	2368074	2396443	69.52%	9.011%
7	7.134	869	875	878	rBV	1902999	2054982	59.61%	7.727%
8	7.851	992	997	1000	rBV	859762	784390	22.75%	2.950%
9	8.933	1175	1181	1184	rBV	2710734	2804567	81.35%	10.546%
10	9.322	1242	1247	1253	rBV	328036	295861	8.58%	1.113%
11	9.598	1289	1294	1298	rBV	939459	831769	24.13%	3.128%
12	10.051	1365	1371	1374	rBV	52707	42421	1.23%	0.160%
13	10.269	1403	1408	1411	rBV2	29732	42029	1.22%	0.158%
14	10.386	1423	1428	1431	rBV	1769164	1818761	52.76%	6.839%
15	10.522	1447	1451	1459	rBV	74996	100157	2.91%	0.377%
16	11.075	1541	1545	1548	rBV	986565	851246	24.69%	3.201%
17	12.274	1747	1749	1753	rVB	58624	55145	1.60%	0.207%
18	12.504	1783	1788	1791	rBV	76194	77561	2.25%	0.292%
19	12.663	1809	1815	1818	rBV	2050760	2078401	60.29%	7.815%
20	13.568	1963	1969	1977	rBV2	115135	151086	4.38%	0.568%
21	13.698	1986	1991	1994	rBV	628750	578914	16.79%	2.177%
22	14.204	2073	2077	2084	rBV2	48887	63433	1.84%	0.239%
23	14.692	2157	2160	2163	rBV	32074	45929	1.33%	0.173%
24	15.068	2219	2224	2230	rVV	421979	504503	14.63%	1.897%
25	16.327	2433	2438	2442	rBV6	17671	35792	1.04%	0.135%
26	17.298	2598	2603	2613	rVB6	45994	112790	3.27%	0.424%
27	17.509	2634	2639	2653	rVB8	84457	278724	8.09%	1.048%

Sum of corrected areas: 26593866

LSC Report - Integrated Chromatogram

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Data File : BF096911.D
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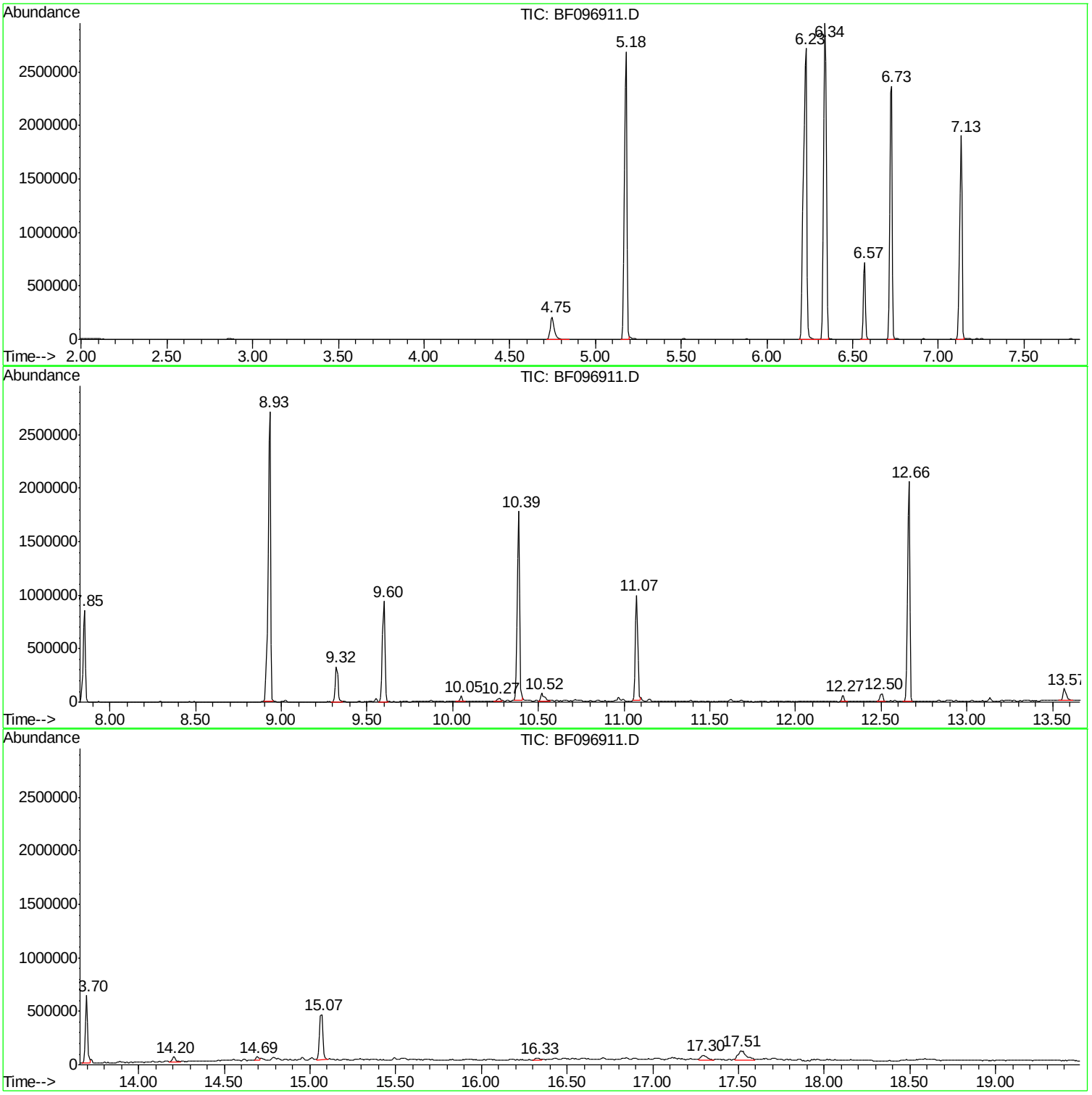
Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-B

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
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Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-B

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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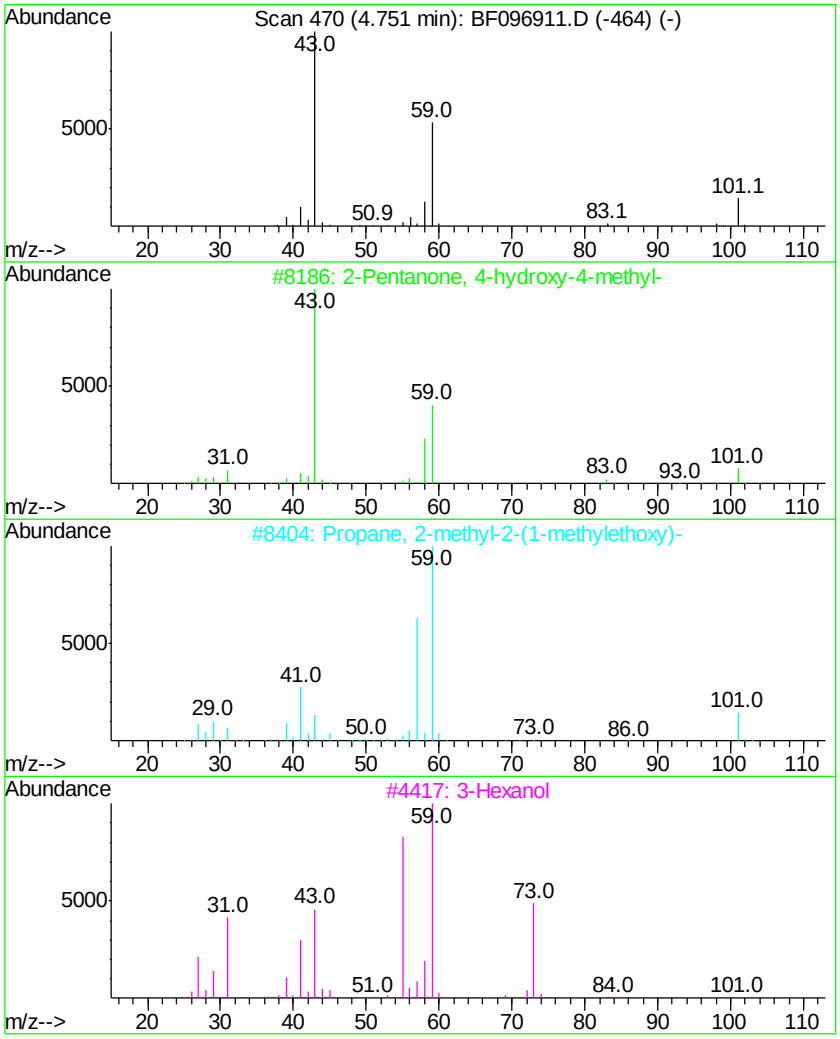
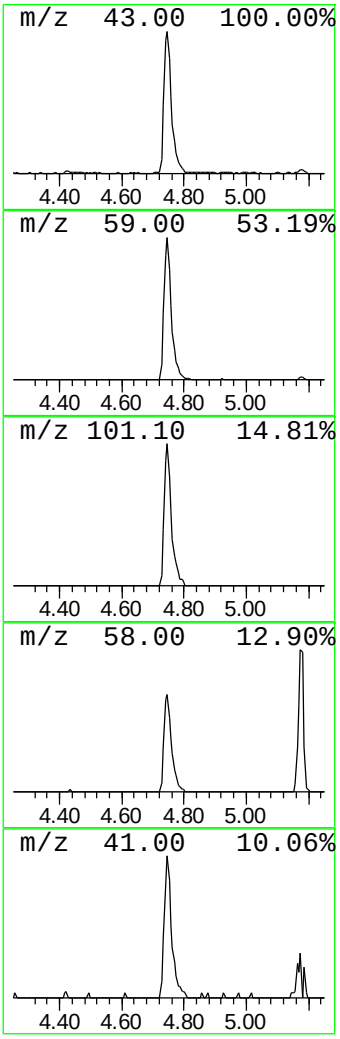
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	10.67 ng	343508	1,4-Dichlorobenzene-d4	6.57

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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28





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Data File : BF096911.D
Acq On : 20 Jul 2017 17:47
Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-B

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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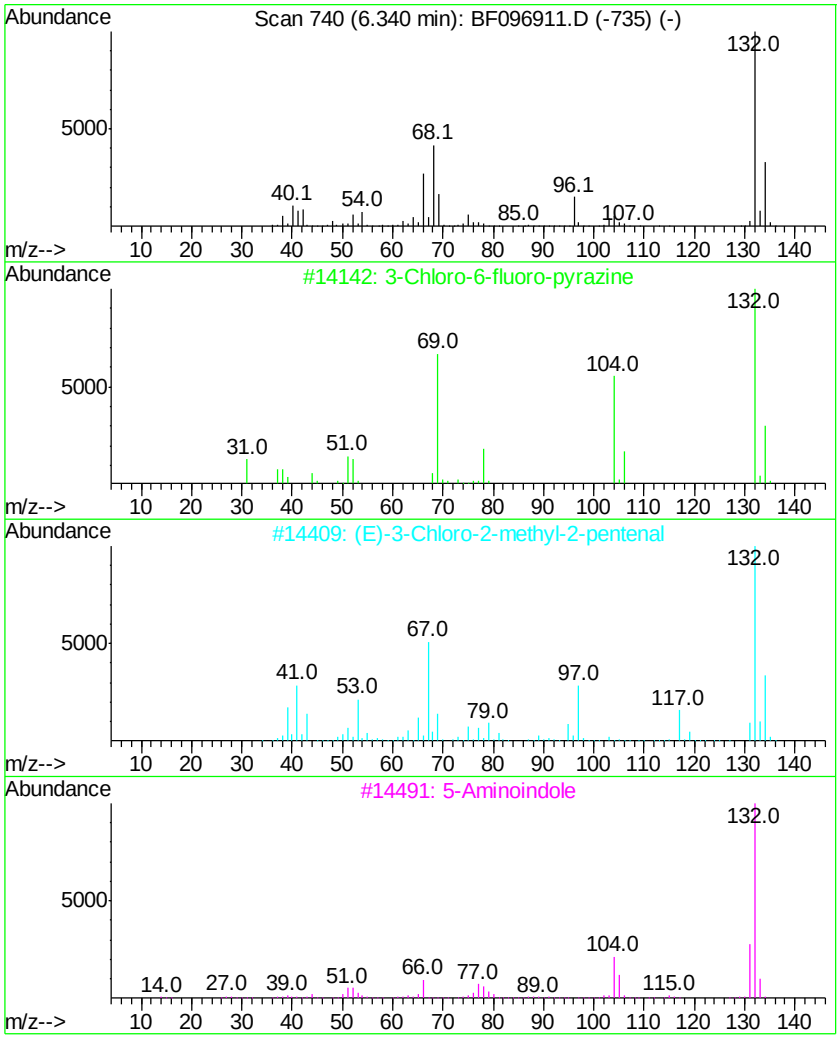
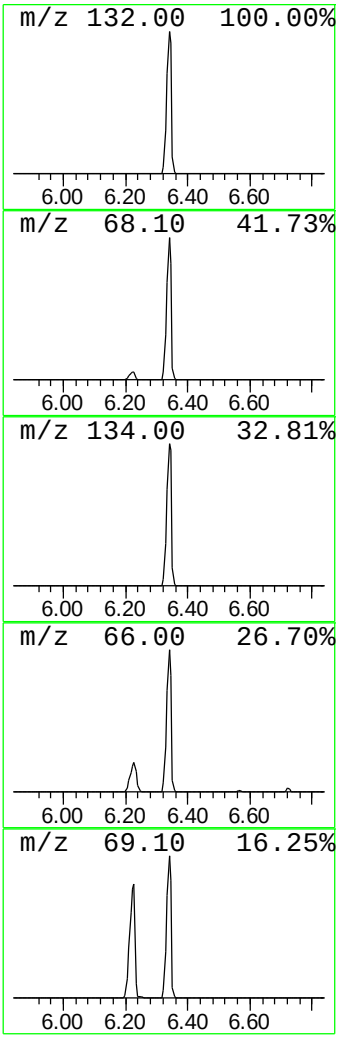
Peak Number 2 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	98.90 ng	3182860	1,4-Dichlorobenzene-d4	6.57

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	27
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





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096911.D
Acq On : 20 Jul 2017 17:47
Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-B

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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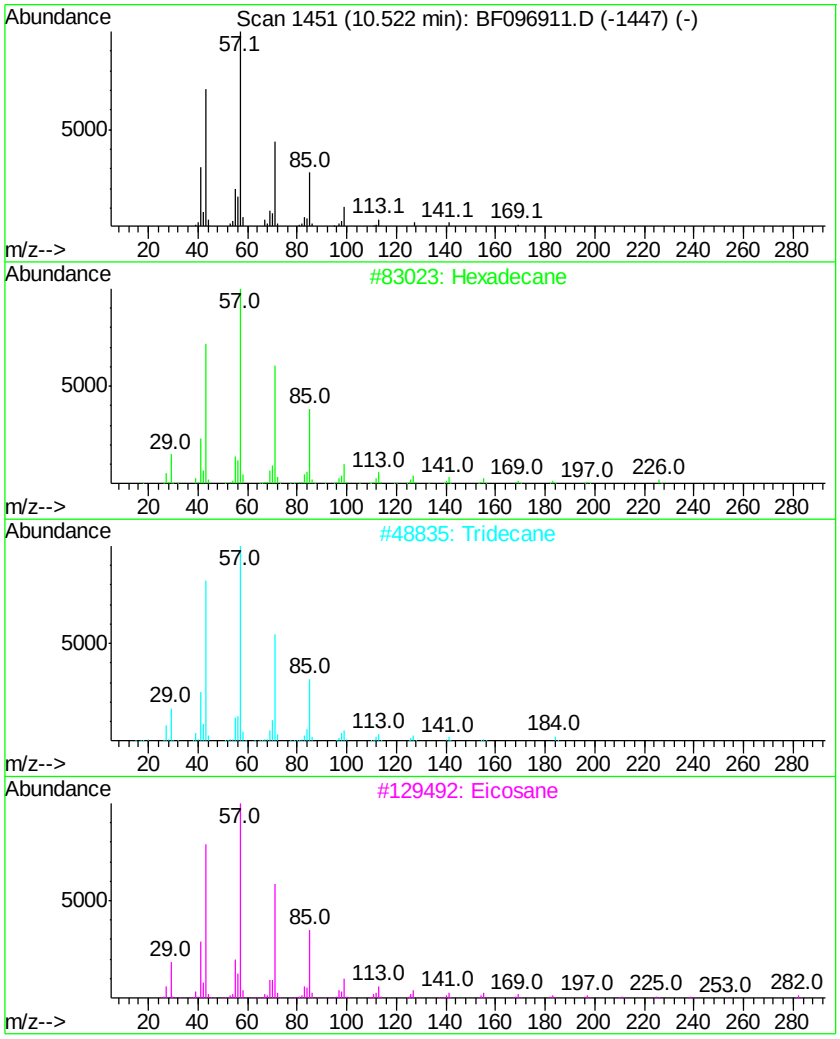
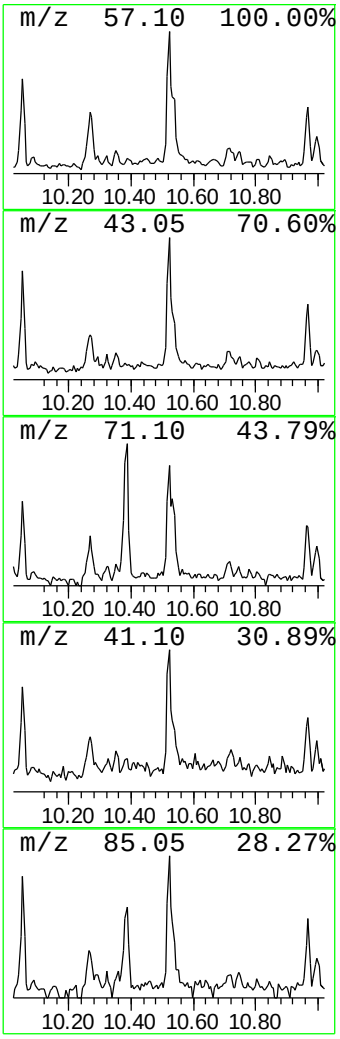
Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	2.35 ng	100157	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Tridecane	184	C13H28	000629-50-5	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Heptadecane	240	C17H36	000629-78-7	80
5	Octacosane	394	C28H58	000630-02-4	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096911.D
Acq On : 20 Jul 2017 17:47
Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-B

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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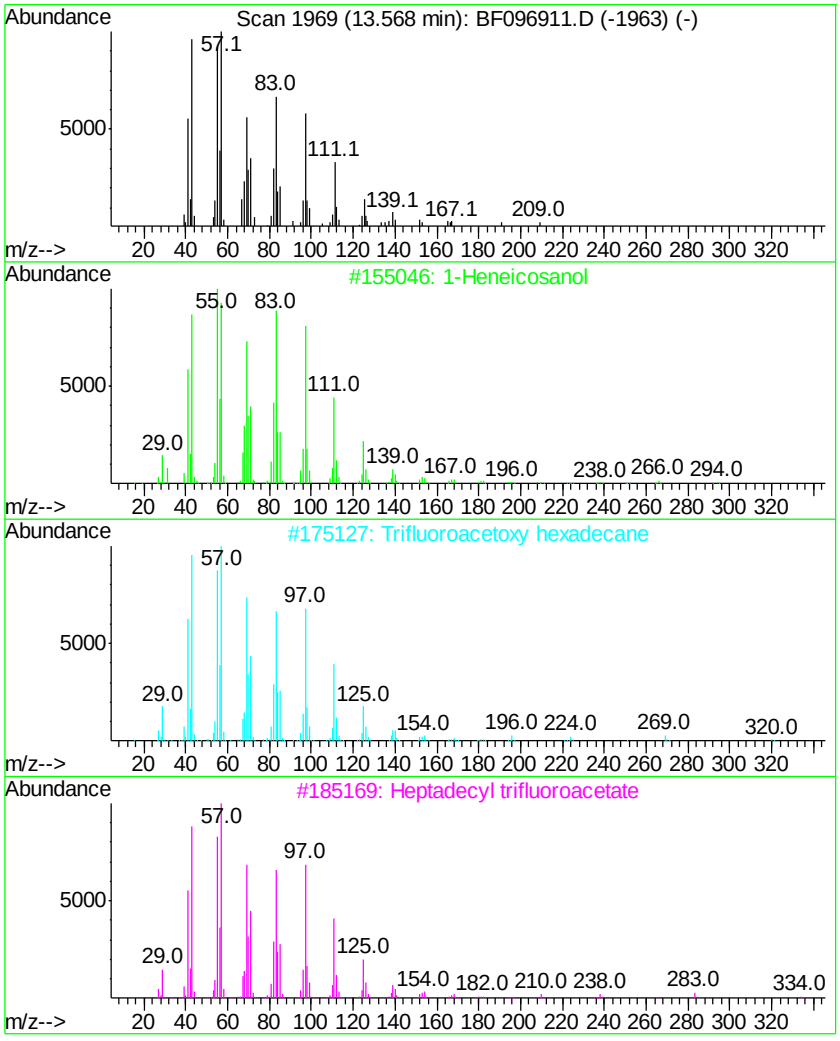
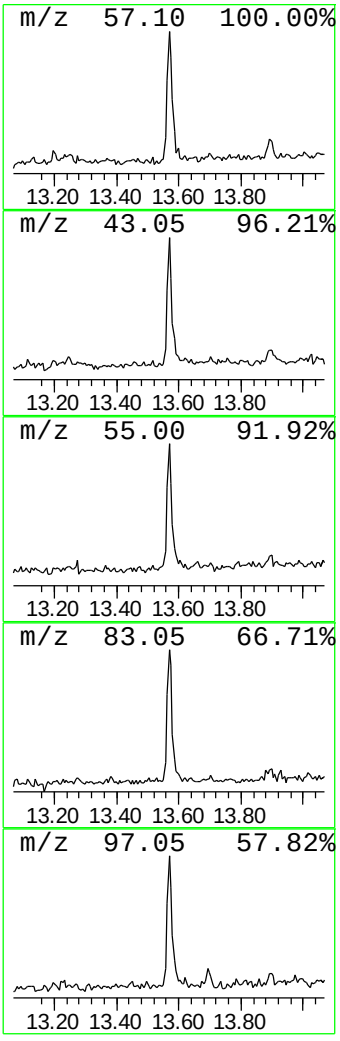
Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	5.22 ng	151086	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096911.D
Acq On : 20 Jul 2017 17:47
Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-B

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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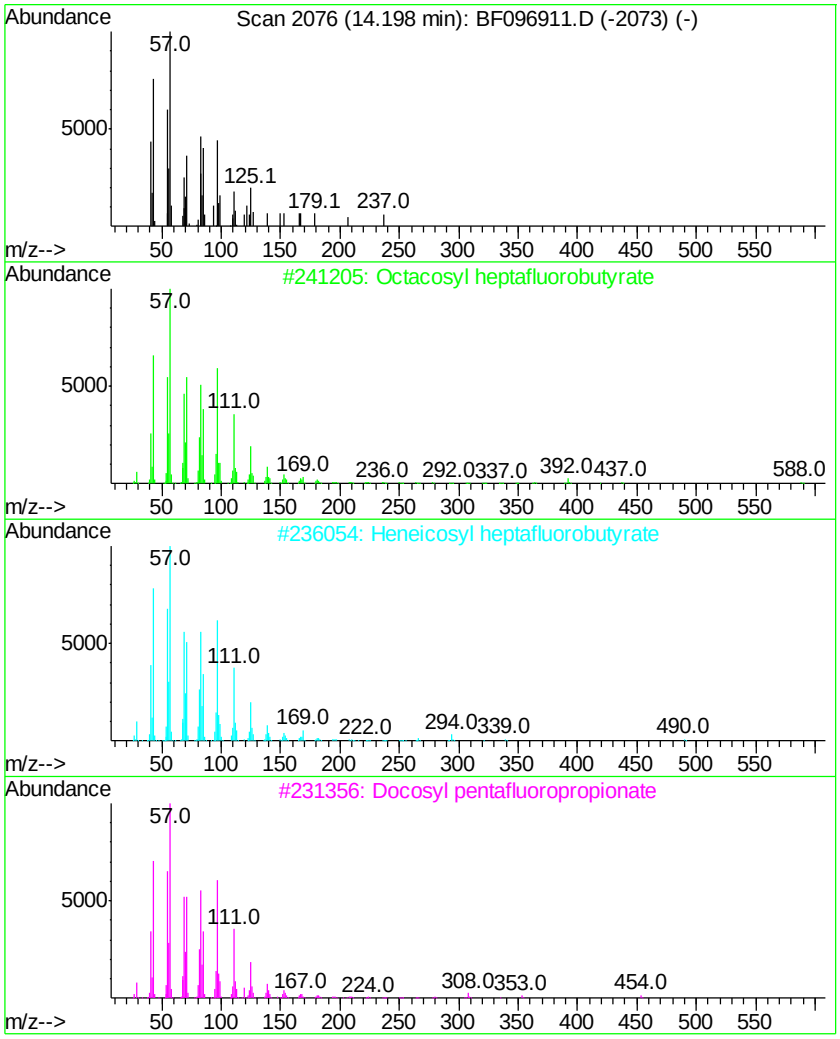
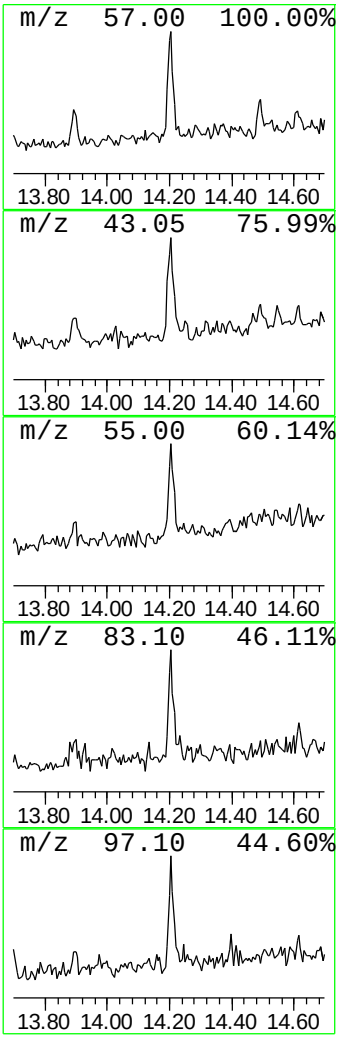
Peak Number 7 Octacosyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	2.19 ng	63433	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	94
2	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
5	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91





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Operator : SJ/JU
Sample : I4282-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-007-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

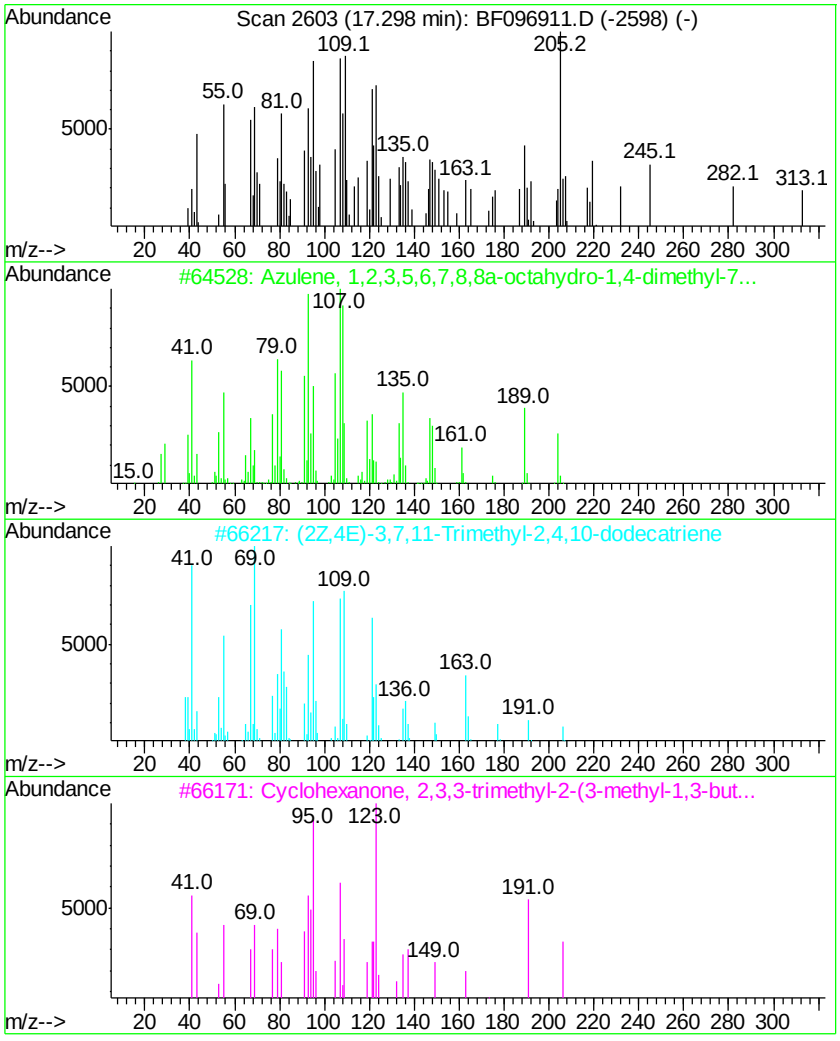
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

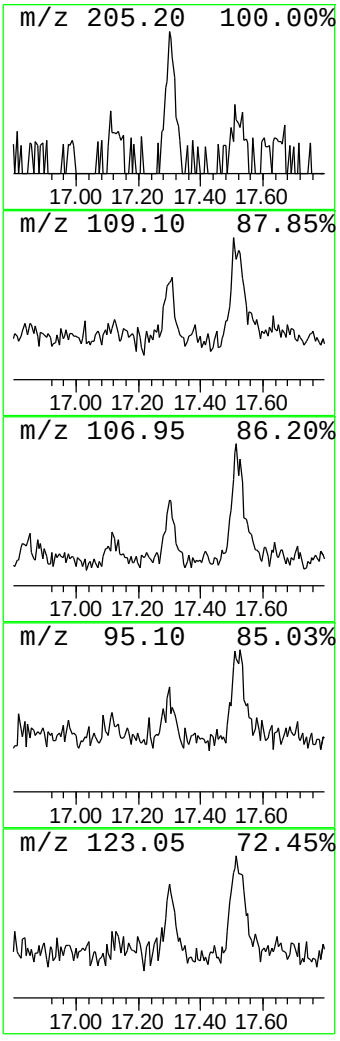
****

Peak Number 8 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	4.47 ng	112790	Perylene-d12	15.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene, 1,2,3,5,6,7,8,8a-octahv...	204	C15H24	003691-11-0	72
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	38
3	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	38
4	2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	38
5	Caparratriene	206	C15H26	1000374-08-7	38





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

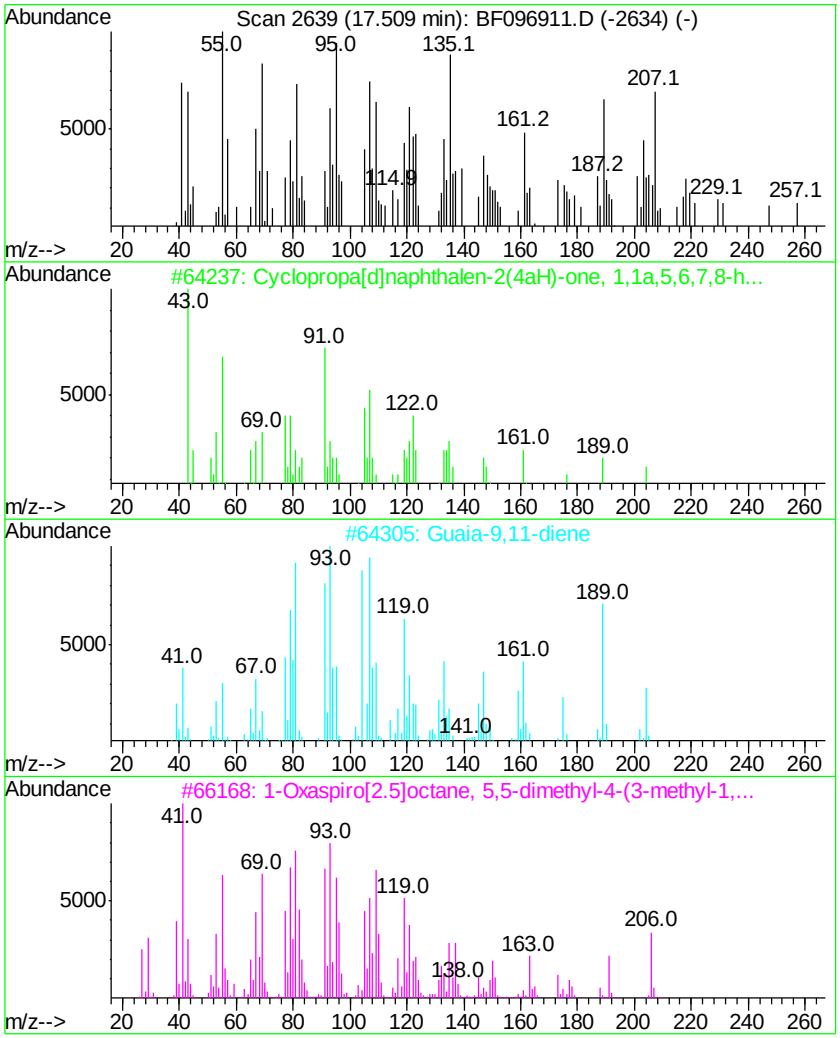
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

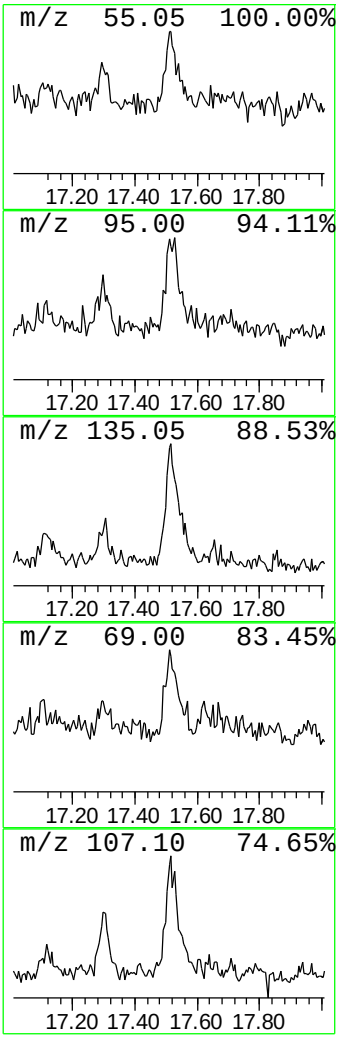
****

Peak Number 9 Cyclopropa[d]naphthalen-2(4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.51	11.05 ng	278724	Perylene-d12	15.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropa[d]naphthalen-2(4aH)-o...	204	C14H20O	004677-90-1	87
2	Guaia-9,11-diene	204	C15H24	1000374-19-8	47
3	1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	44
4	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	42
5	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
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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...	4.75	10.7	ng	343508	1	6.57	643632	20.0
unknown6.34	6.34	98.9	ng	3182860	1	6.57	643632	20.0
Hexadecane	10.52	2.4	ng	100157	4	11.07	851246	20.0
1-Heneicosanol	13.57	5.2	ng	151086	5	13.70	578914	20.0
Octacosyl heptafl...	14.20	2.2	ng	63433	5	13.70	578914	20.0
Azulene, 1,2,3,5,...	17.30	4.5	ng	112790	6	15.07	504503	20.0
Cyclopropa[d]naph...	17.51	11.1	ng	278724	6	15.07	504503	20.0