LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106657.D
Acq On : 21 Jun 2018 13:12
Operator : JU/SJ
Sample : J3584-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

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-BF061918.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	rBV	140304	167932	7.96%	0.883%
2	5.601	551	555	566	rBV	1885164	1746050	82.74%	9.176%
3	6.607	721	726	731	rBV	1851058	1862542	88.26%	9.788%
4	6.736	744	748	751	rBV	1947523	1841116	87.25%	9.676%
5	6.960	782	786	789	rBV	726945	566096	26.83%	2.975%
6	7.119	808	813	816	rBV	1641576	1444743	68.46%	7.593%
7	7.525	877	882	885	rBV	1325946	1240982	58.81%	6.522%
8	8.242	1000	1004	1008	rBV	920238	734633	34.81%	3.861%
9	9.319	1182	1187	1190	rBV	2420716	2110262	100.00%	11.090%
10	9.707	1250	1253	1260	rVB	342115	270631	12.82%	1.422%
11	9.913	1285	1288	1293	rBV	45648	36936	1.75%	0.194%
12	10.001	1299	1303	1307	rBV2	978219	821742	38.94%	4.318%
13	10.413	1371	1373	1376	rVB	60215	41609	1.97%	0.219%
14	10.795	1434	1438	1441	rBV	1516688	1358223	64.36%	7.138%
15	10.883	1450	1453	1461	rVB	47531	51255	2.43%	0.269%
16	11.495	1553	1557	1560	rBV	923109	768560	36.42%	4.039%
17	13.077	1822	1826	1829	rBV	2129078	1960024	92.88%	10.300%
18	13.630	1916	1920	1923	rBV2	37016	34082	1.62%	0.179%
19	13.959	1972	1976	1985	rBV	156440	175996	8.34%	0.925%
20	14.148	2004	2008	2016	rVB	759017	701189	33.23%	3.685%
21	14.283	2028	2031	2035	rBV	58586	55242	2.62%	0.290%
22	14.601	2082	2085	2092	rBV3	85697	106374	5.04%	0.559%
23	14.924	2136	2140	2143	rVB	71095	77046	3.65%	0.405%
24	15.001	2150	2153	2159	rVB	99271	105223	4.99%	0.553%
25	15.277	2197	2200	2207	rVB	73707	85909	4.07%	0.451%
26	15.689	2264	2270	2278	rBV	449403	612112	29.01%	3.217%
27	16.142	2344	2347	2352	rVB2	36031	51940	2.46%	0.273%

Sum of corrected areas: 19028449

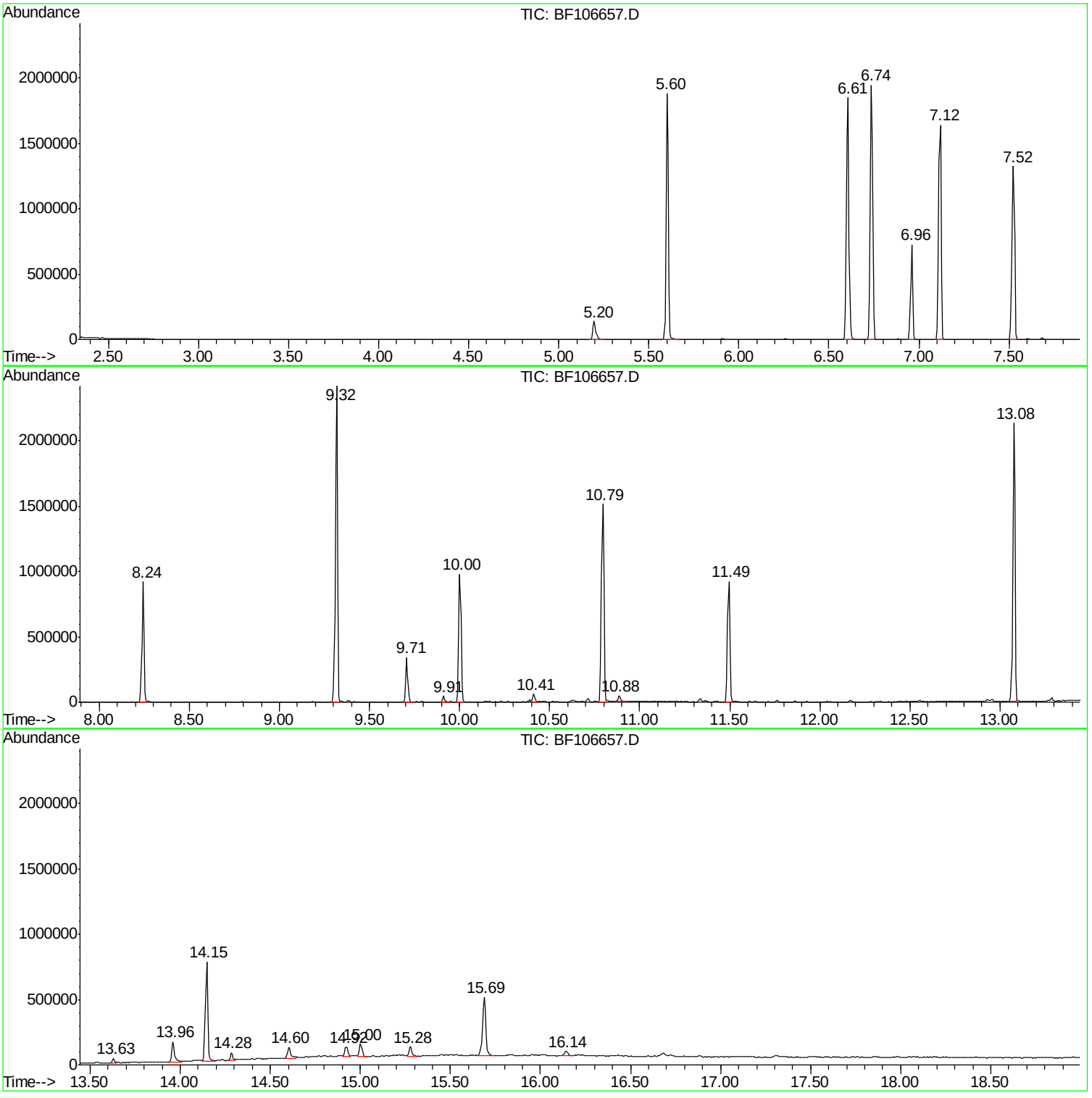
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106657.D
Acq On : 21 Jun 2018 13:12
Operator : JU/SJ
Sample : J3584-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF062118\
Data File : BF106657.D
Acq On : 21 Jun 2018 13:12
Operator : JU/SJ
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

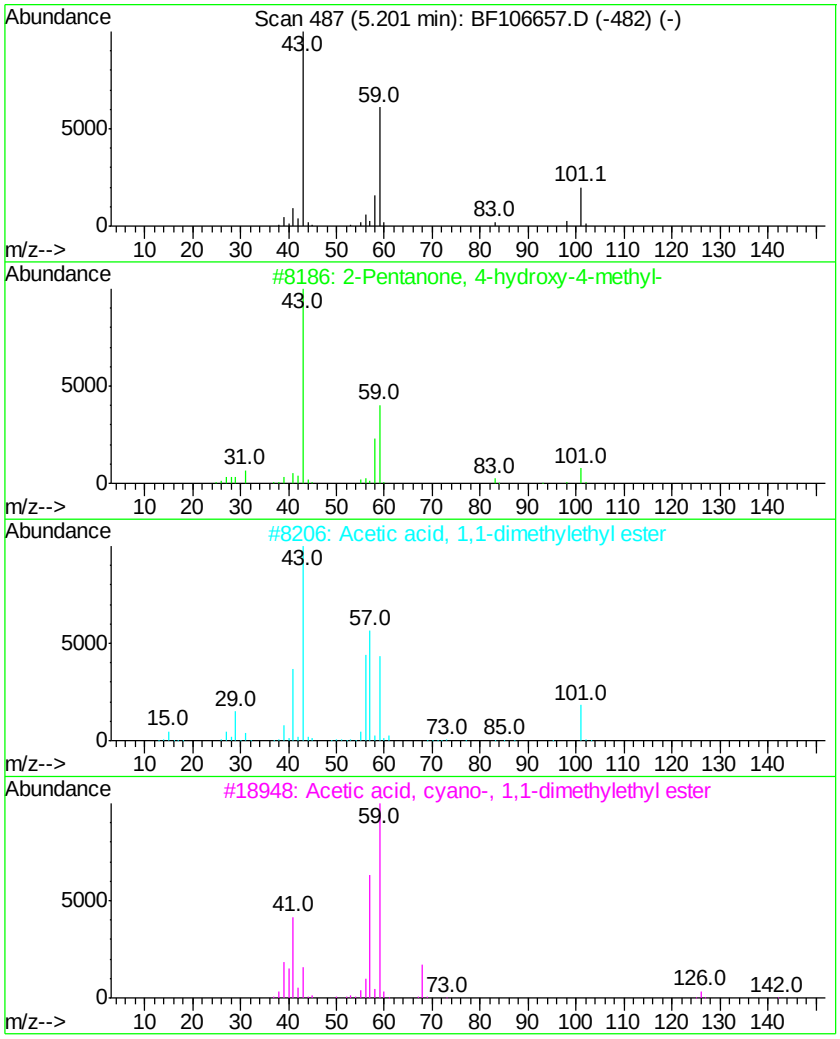
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

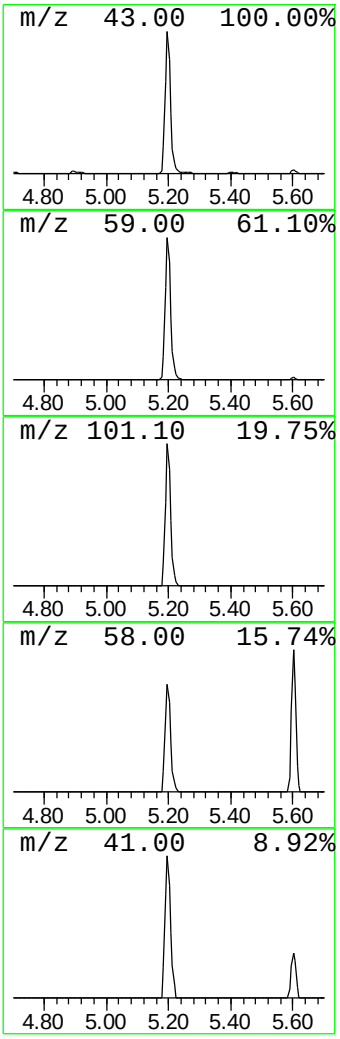
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.93 ng	167932	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Data File : BF106657.D
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Operator : JU/SJ
Sample : J3584-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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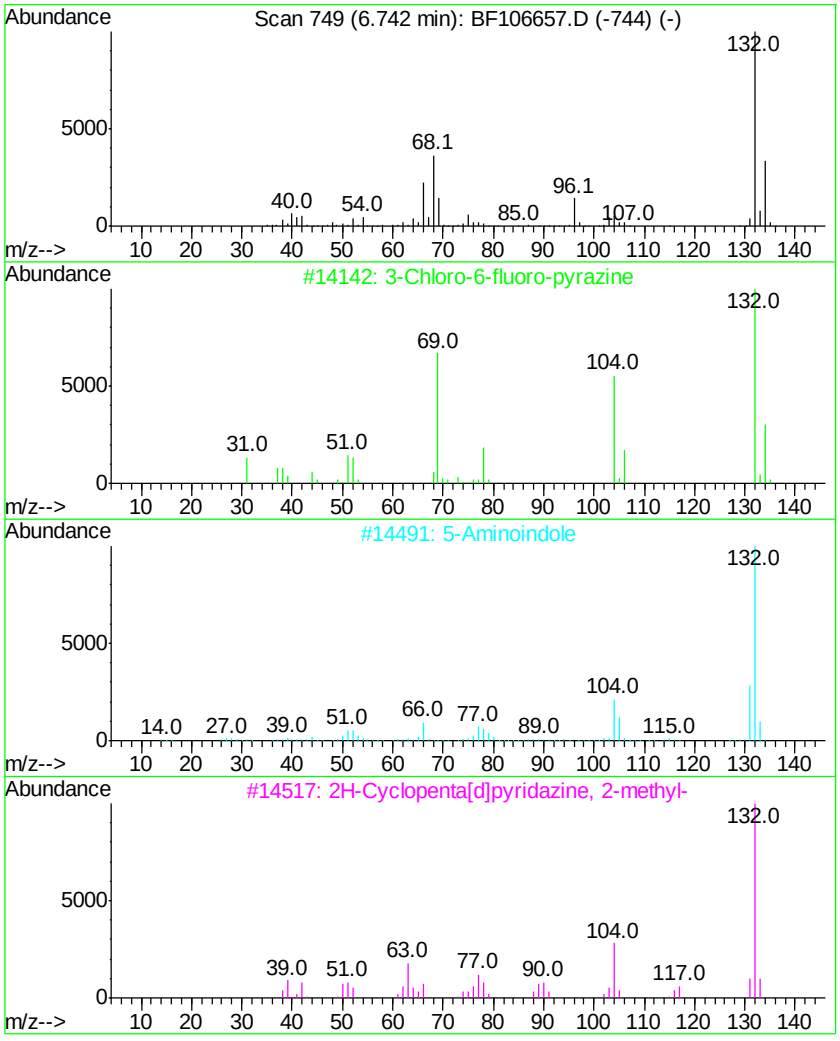
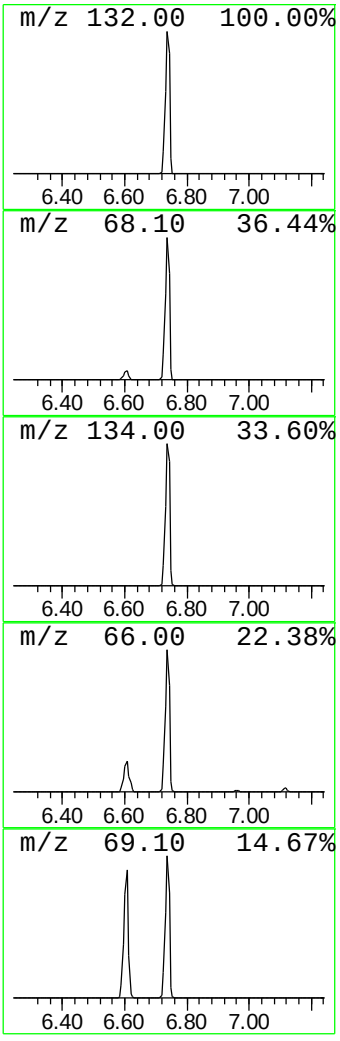
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	65.05 ng	1841120	1,4-Dichlorobenzene-d4	6.96

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106657.D
Acq On : 21 Jun 2018 13:12
Operator : JU/SJ
Sample : J3584-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

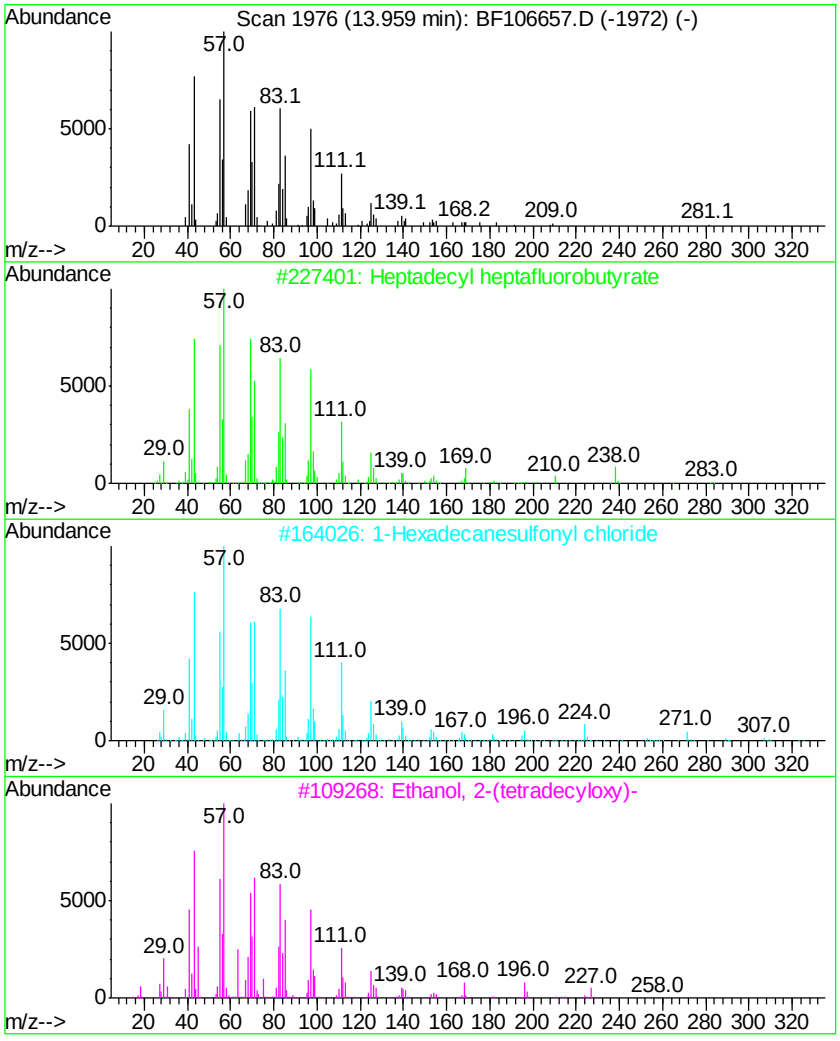
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

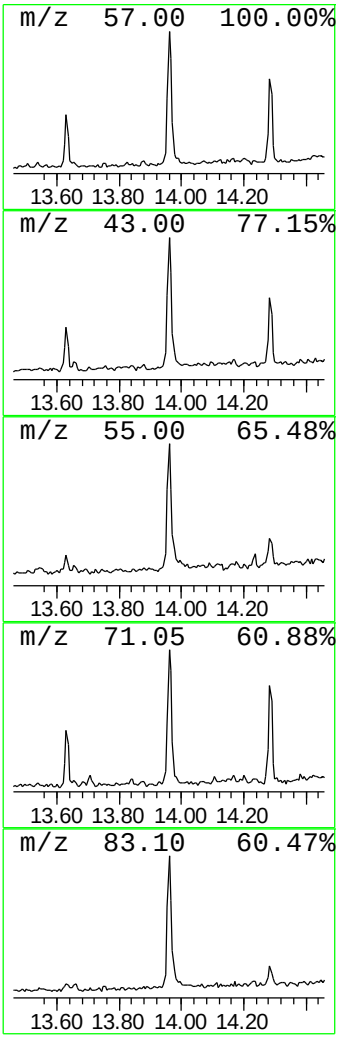
****

Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.02 ng	175996	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	90





Library Search Compound Report

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Data File : BF106657.D
Acq On : 21 Jun 2018 13:12
Operator : JU/SJ
Sample : J3584-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

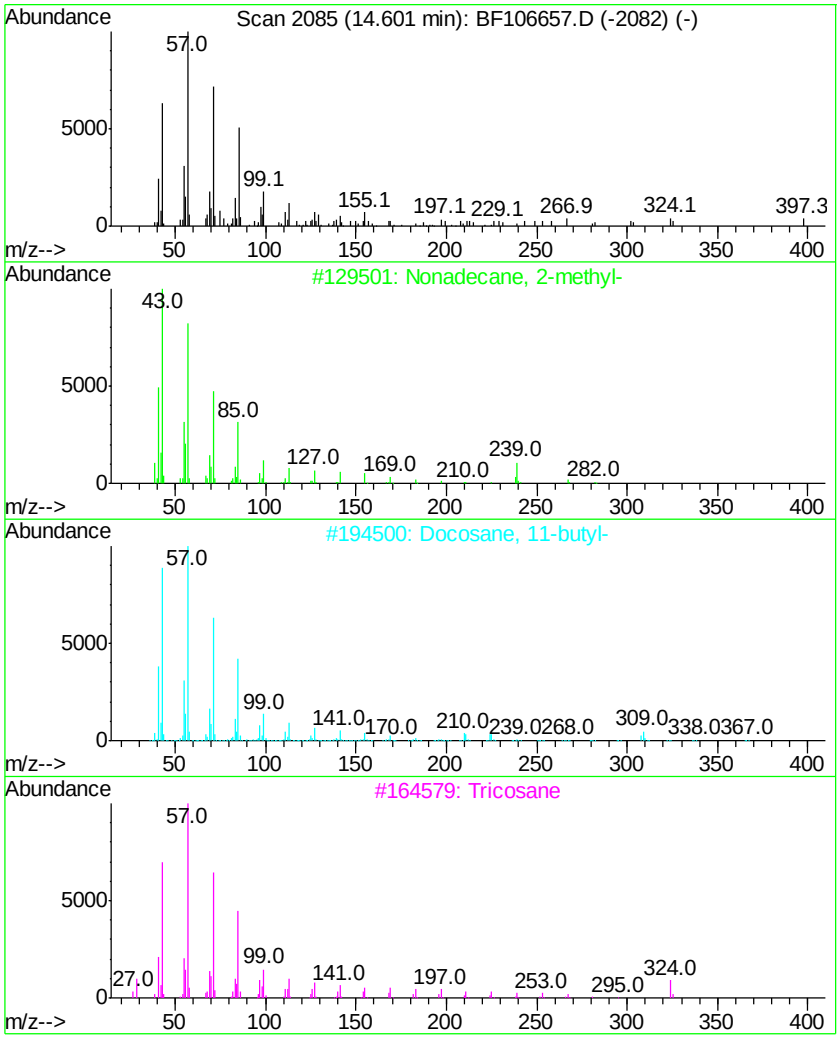
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

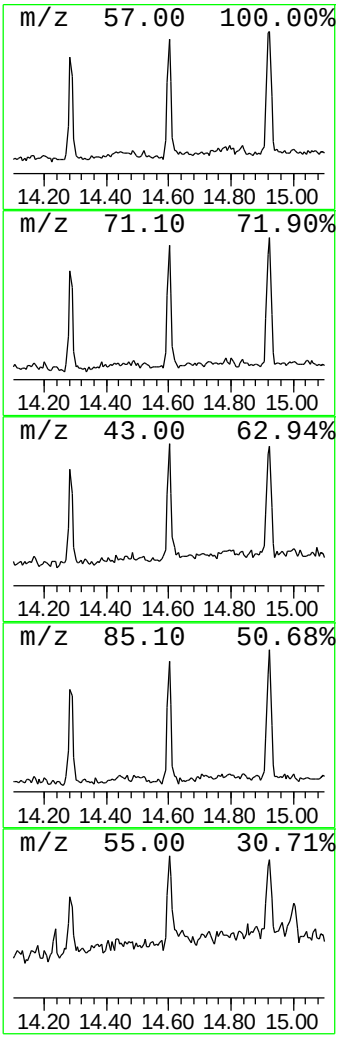
****

Peak Number 5 Nonadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.03 ng	106374	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	93
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
3	Tricosane	324	C23H48	000638-67-5	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Hexadecane	226	C16H34	000544-76-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
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Acq On : 21 Jun 2018 13:12
Operator : JU/SJ
Sample : J3584-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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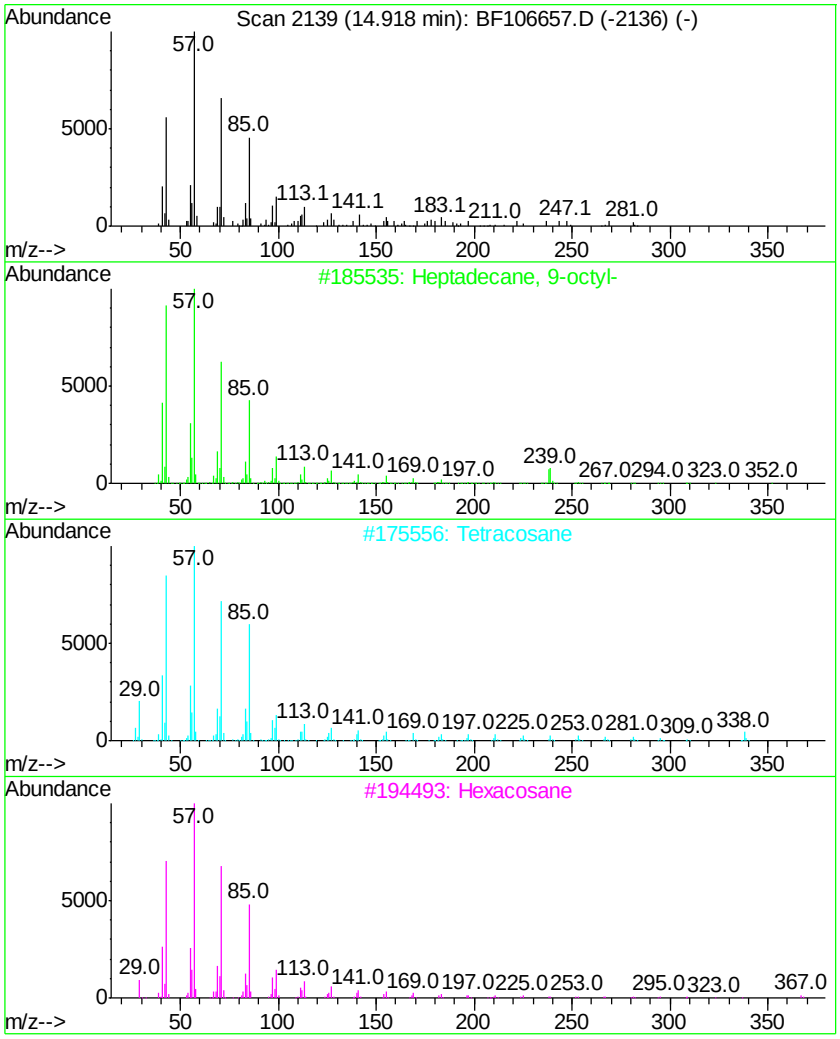
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

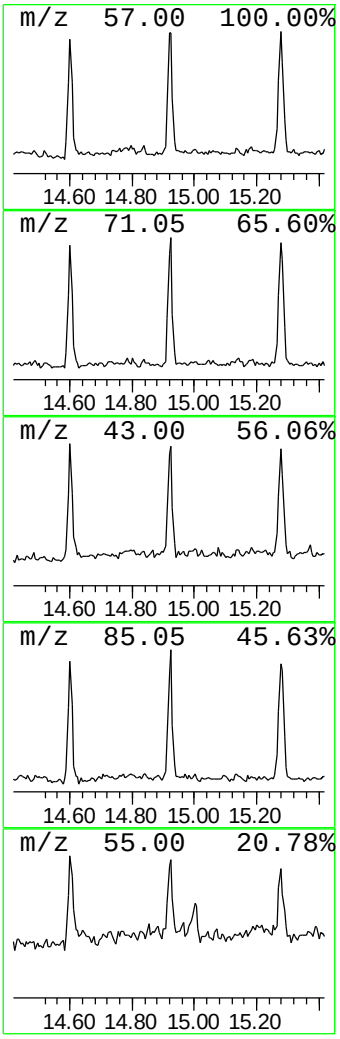
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.52 ng	77046	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
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Sample : J3584-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

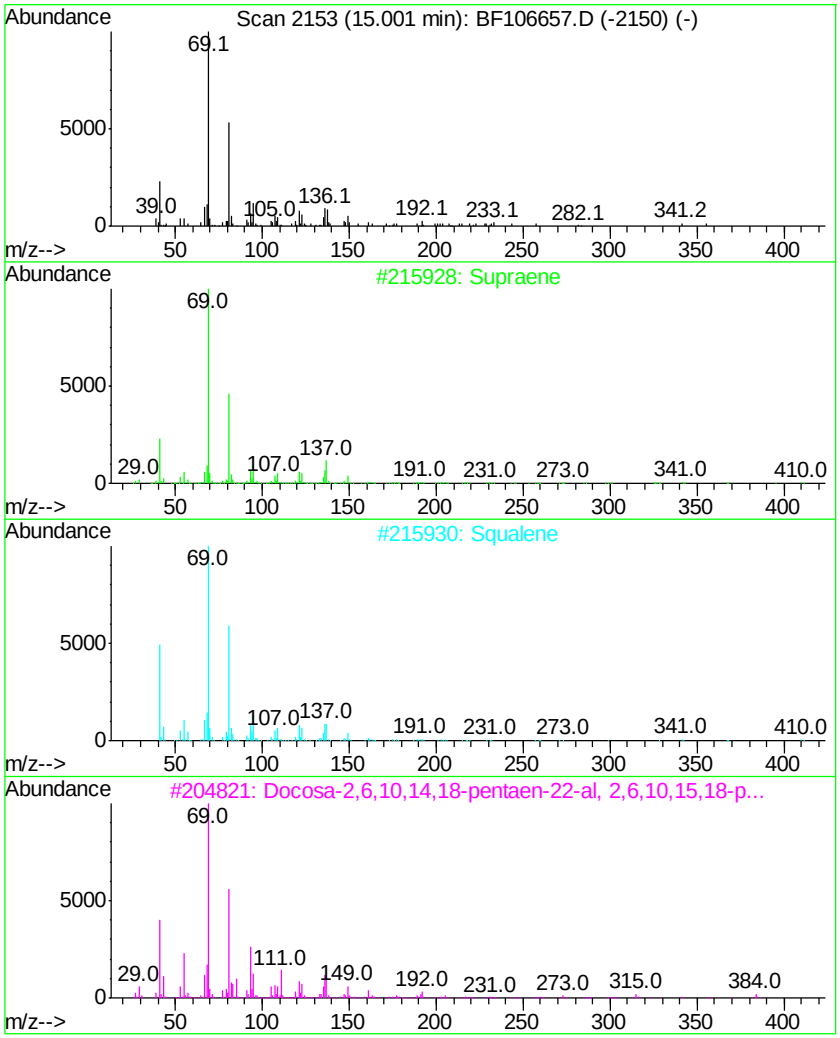
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

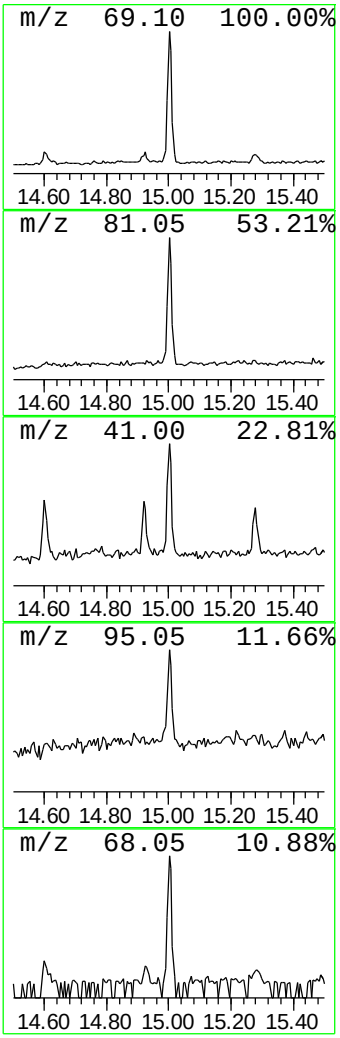
****

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	3.44 ng	105223	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	86
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4	trans-Farnesol	222	C15H26O	000106-28-5	72
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64





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Misc :
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ClientSampleId : TP-12-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

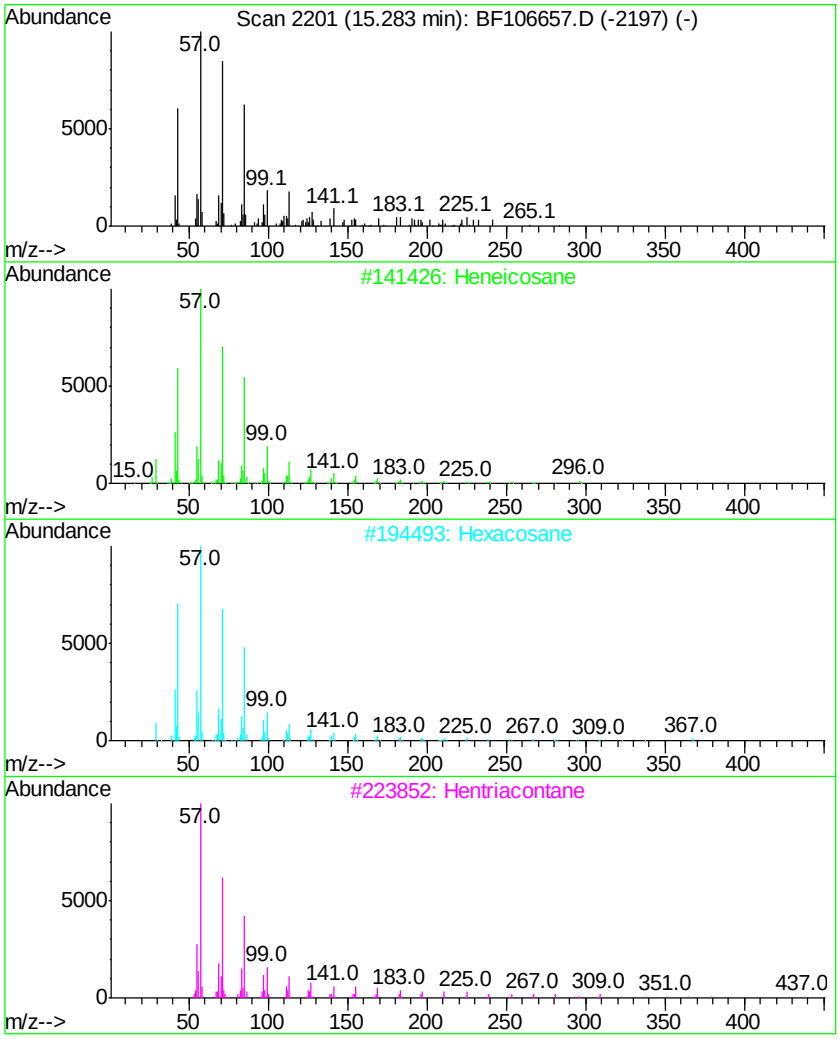
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

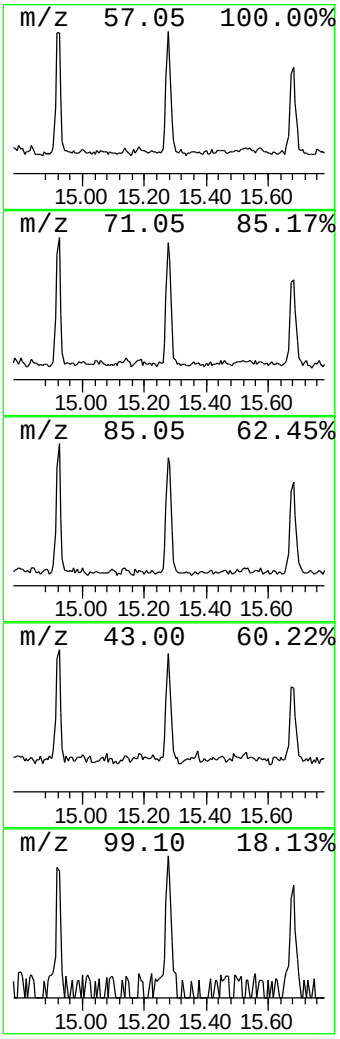
****

Peak Number 8 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.81 ng	85909	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Docosane	310	C22H46	000629-97-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062118\
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Instrument : BNA_F
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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...	5.20	5.9	ng	167932	1	6.96	566096	20.0
unknown6.74	6.74	65.0	ng	1841120	1	6.96	566096	20.0
Heptadecyl heptaf...	13.96	5.0	ng	175996	5	14.15	701189	20.0
Nonadecane, 2-met...	14.60	3.0	ng	106374	5	14.15	701189	20.0
Heptadecane, 9-oc...	14.92	2.5	ng	77046	6	15.69	612112	20.0
Supraene	15.00	3.4	ng	105223	6	15.69	612112	20.0
Heneicosane	15.28	2.8	ng	85909	6	15.69	612112	20.0