LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

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-BF040618.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	510	rVB	142467	207883	5.12%	0.590%
2	5.422	560	567	569	rBV	3271516	3863458	95.16%	10.965%
3	5.745	618	622	629	rVB	85625	72283	1.78%	0.205%
4	6.022	666	669	673	rBV	52254	47256	1.16%	0.134%
5	6.069	673	677	688	rVB	118687	210868	5.19%	0.598%
6	6.439	732	740	743	rBV	3321625	3890835	95.83%	11.043%
7	6.575	758	763	766	rBV	3711292	3934892	96.92%	11.168%
8	6.804	798	802	805	rBV	1072756	835094	20.57%	2.370%
9	6.963	824	829	832	rVB	3301324	3010742	74.16%	8.545%
10	7.369	892	898	901	rBV	2222314	2535287	62.44%	7.196%
11	8.086	1016	1020	1023	rBV	1434205	1123115	27.66%	3.188%
12	9.169	1198	1204	1207	rBV	3914414	4060034	100.00%	11.523%
13	9.557	1266	1270	1273	rBV	543963	404951	9.97%	1.149%
14	9.769	1303	1306	1309	rBV	83630	69829	1.72%	0.198%
15	9.839	1314	1318	1322	rVB	1301026	1210515	29.82%	3.436%
16	10.275	1389	1392	1394	rVB	123471	97801	2.41%	0.278%
17	10.492	1423	1429	1432	rBV	38673	49171	1.21%	0.140%
18	10.633	1447	1453	1456	rBV	2625414	2487789	61.28%	7.061%
19	10.745	1469	1472	1481	rBV	116201	122776	3.02%	0.348%
20	11.192	1545	1548	1551	rBV	53307	47471	1.17%	0.135%
21	11.327	1567	1571	1574	rBV	1298247	1088460	26.81%	3.089%
22	11.857	1658	1661	1670	rBV2	304245	317258	7.81%	0.900%
23	12.410	1752	1755	1757	rBV	71151	58685	1.45%	0.167%
24	12.639	1791	1794	1799	rBV	38522	43683	1.08%	0.124%
25	12.921	1837	1842	1845	rBV	3187301	3054859	75.24%	8.670%
26	13.810	1990	1993	2005	rBV	490762	478257	11.78%	1.357%
27	13.968	2015	2020	2023	rBV	892675	790724	19.48%	2.244%
28	14.451	2098	2102	2107	rBV3	66827	84568	2.08%	0.240%
29	15.004	2193	2196	2205	rVB	24367	44942	1.11%	0.128%
30	15.086	2207	2210	2213	rBV	37594	42055	1.04%	0.119%
31	15.427	2263	2268	2273	rBV	665649	827198	20.37%	2.348%
32	15.945	2351	2356	2362	rBV	75888	121146	2.98%	0.344%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 35233885

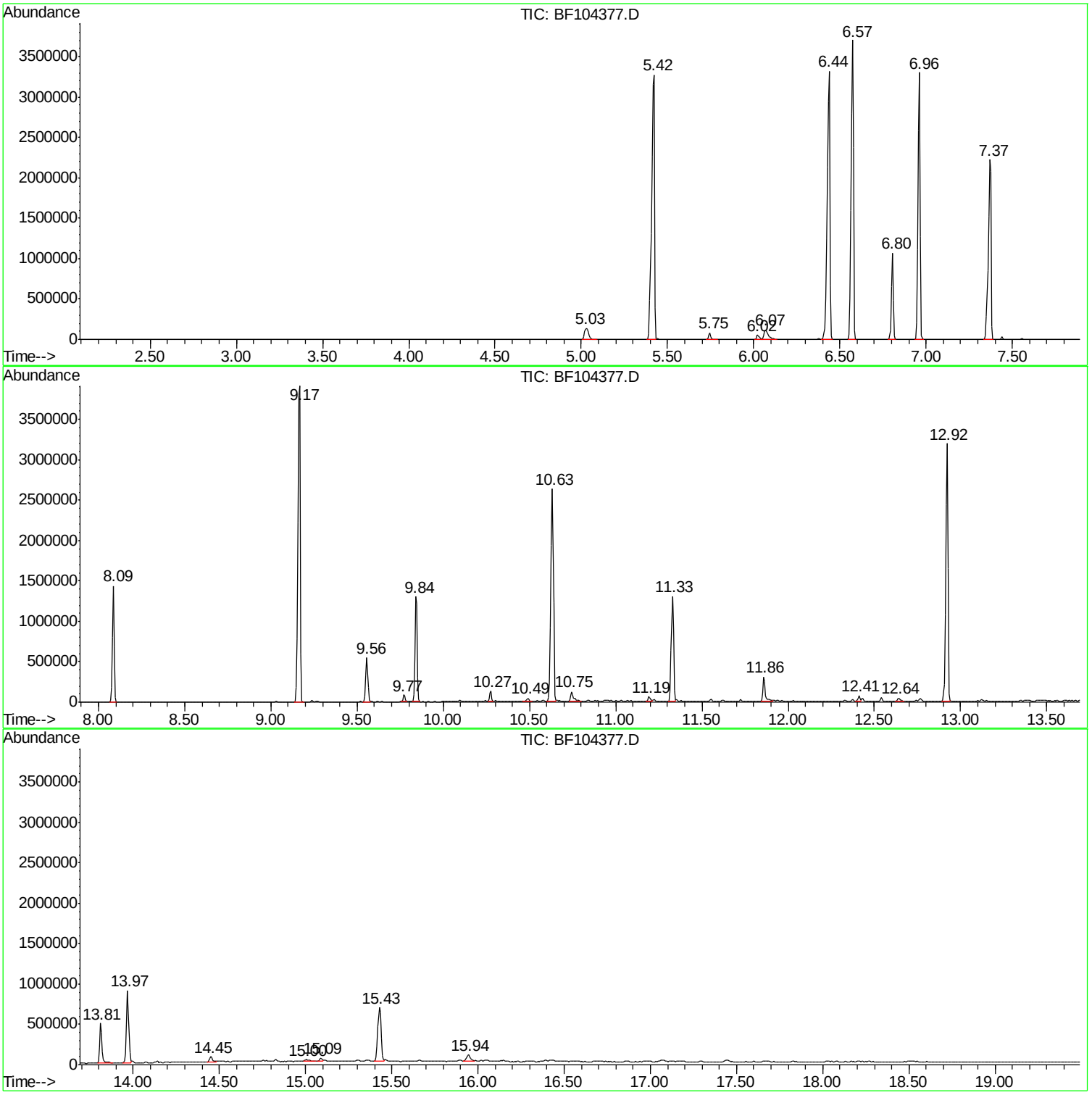
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

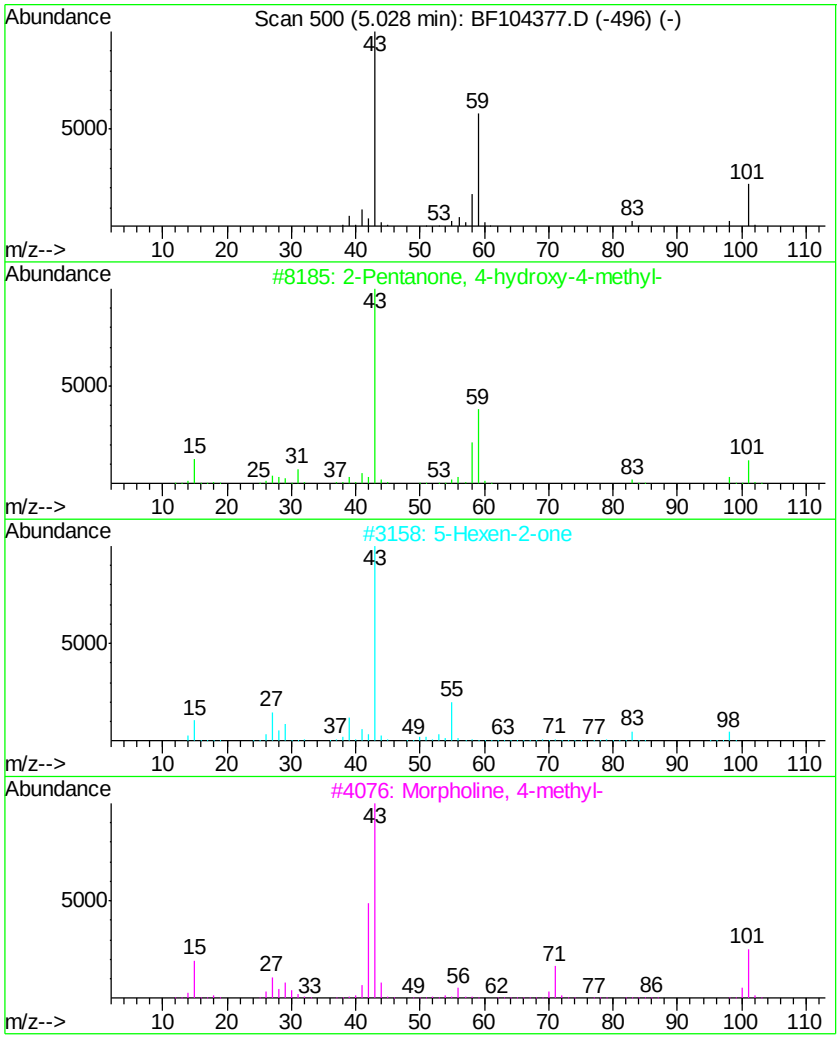
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

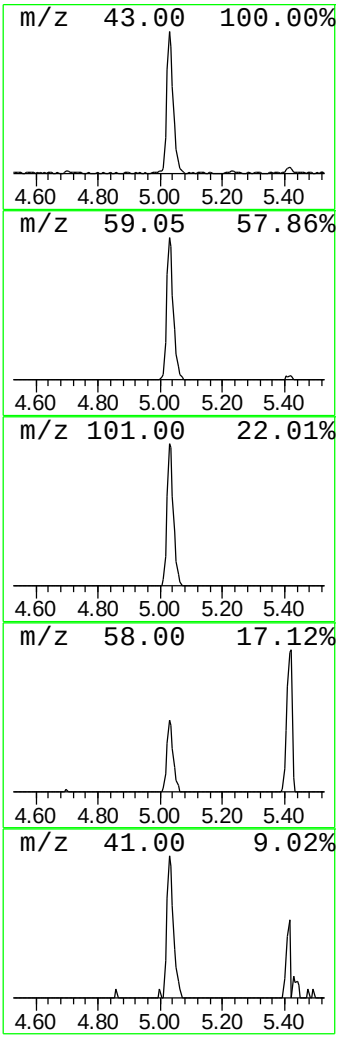
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	4.98 ng	207883	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

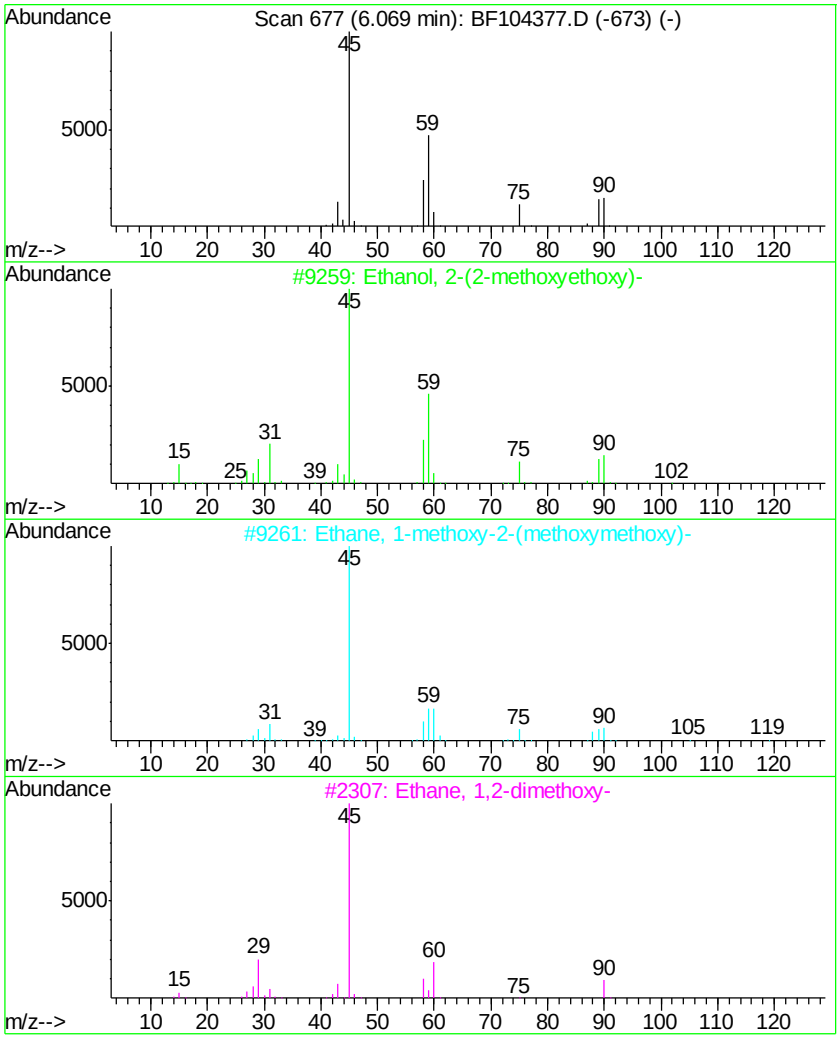
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

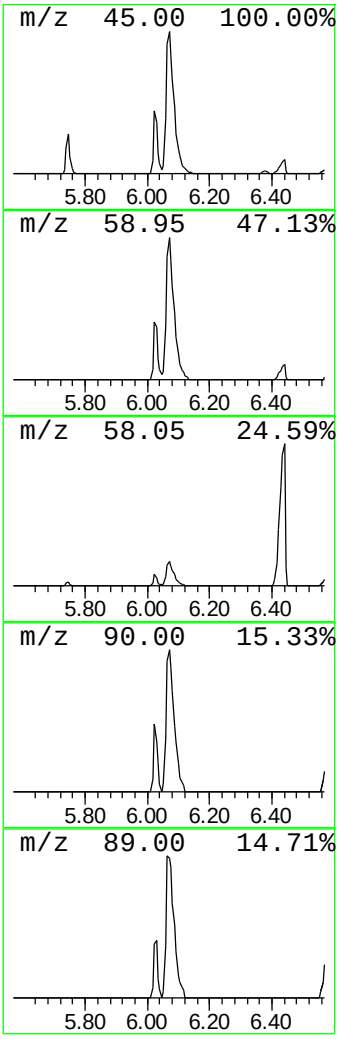
****

Peak Number 2 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.07	5.05 ng	210868	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	90
2	Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	64
3	Ethane, 1,2-dimethoxy-	90	C4H10O2	000110-71-4	47
4	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	36
5	Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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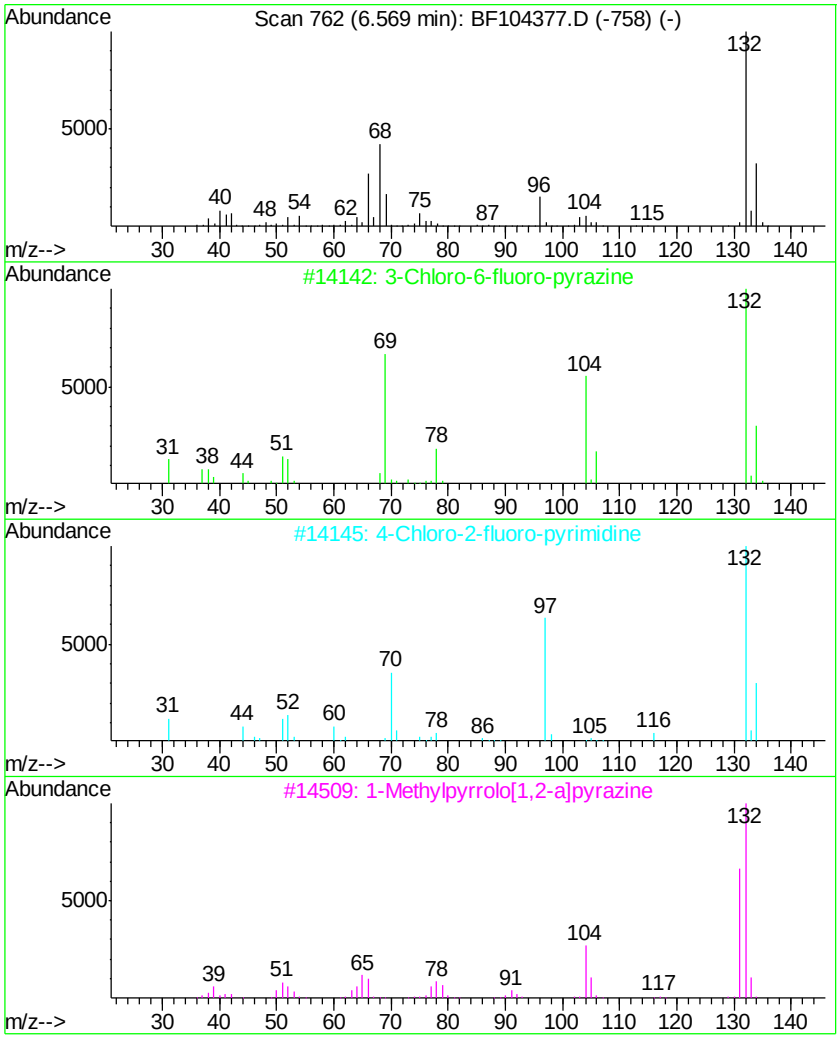
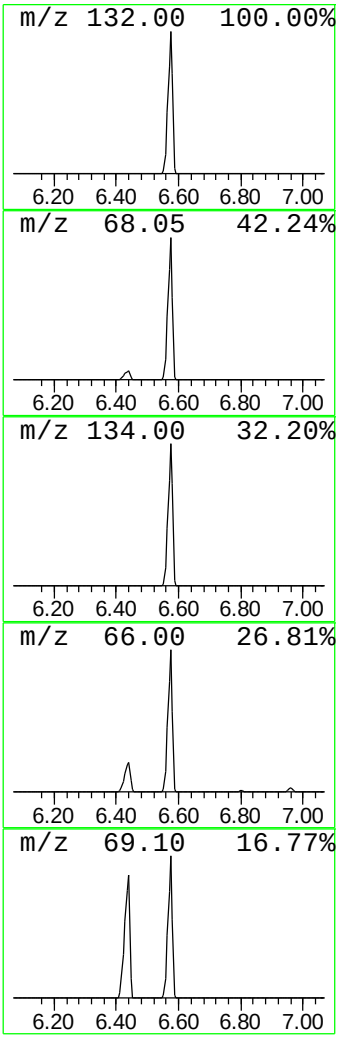
Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	94.24 ng	3934890	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

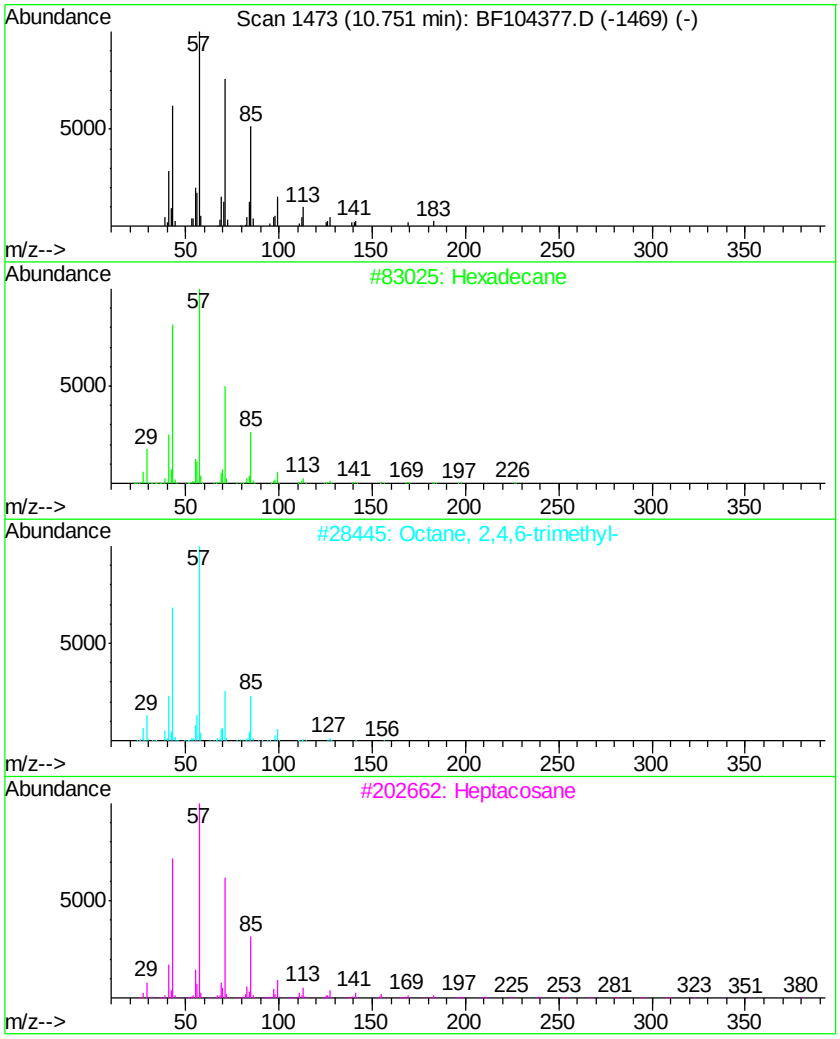
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

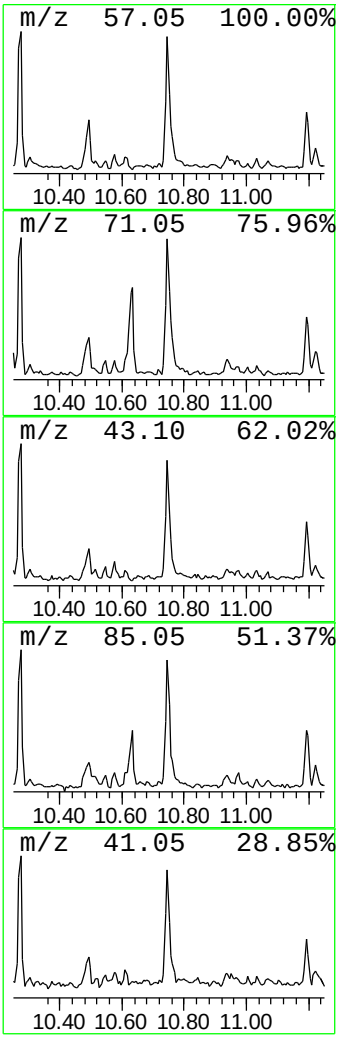
****

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.26 ng	122776	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	86
3	Heptacosane	380	C27H56	000593-49-7	86
4	Tetradecane	198	C14H30	000629-59-4	86
5	Pentadecane	212	C15H32	000629-62-9	86





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Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

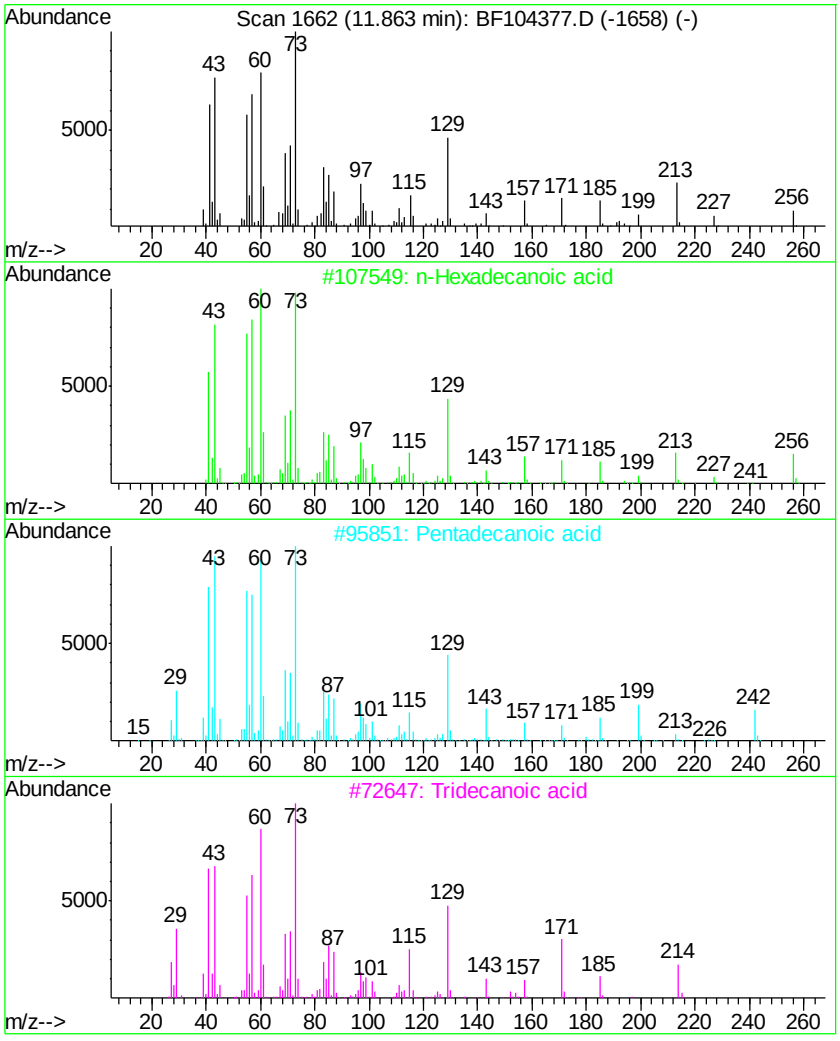
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

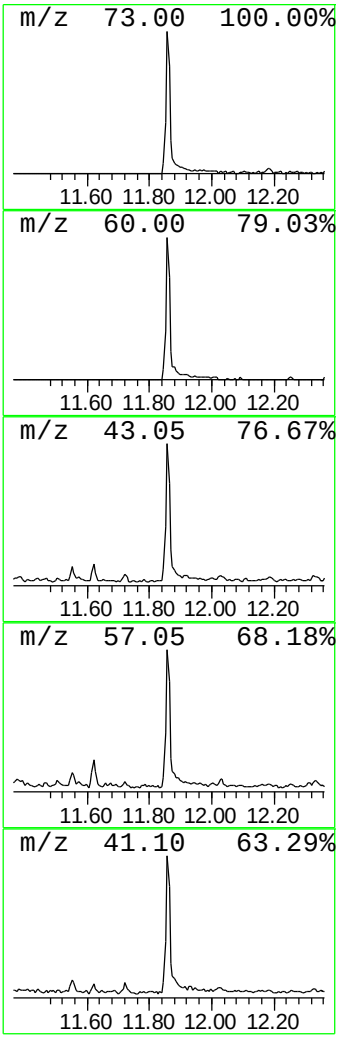
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	5.83 ng	317258	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25





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Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

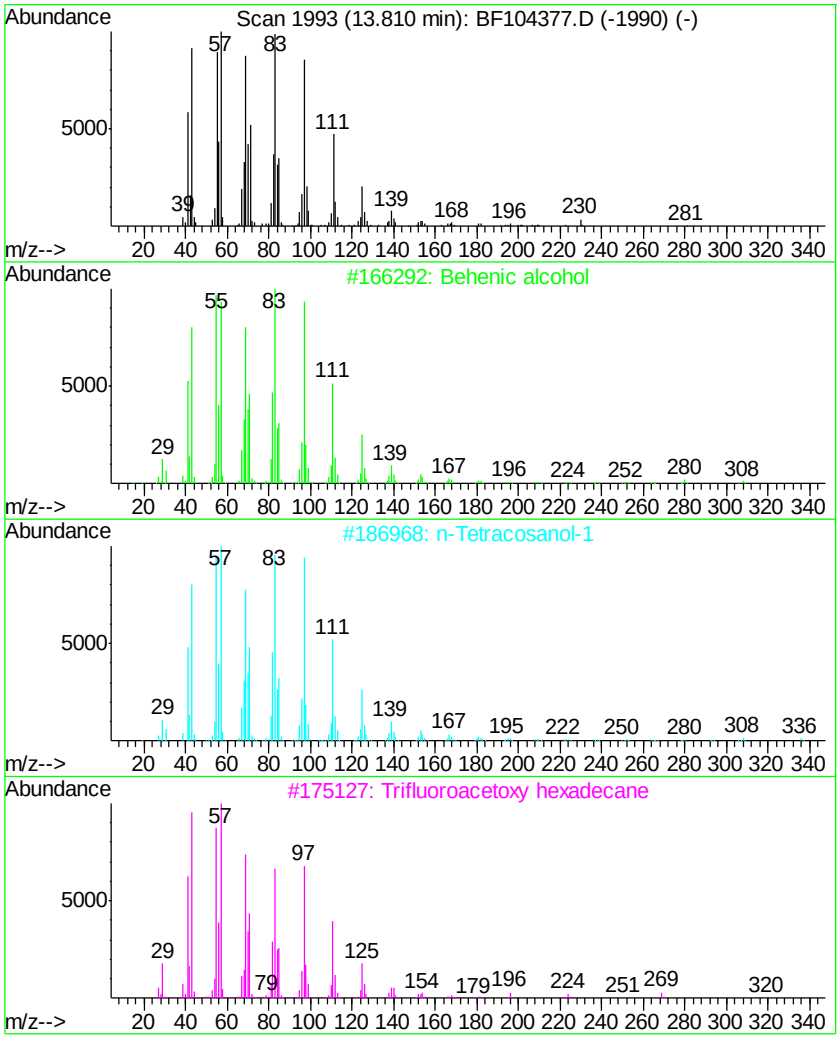
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

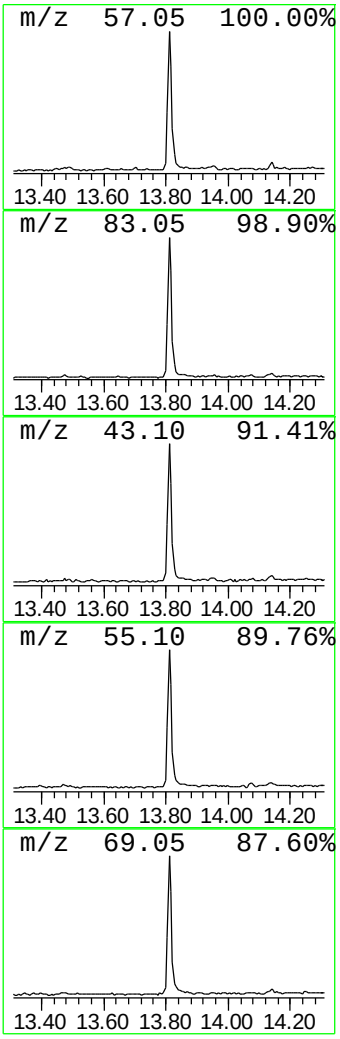
****

Peak Number 7 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	12.10 ng	478257	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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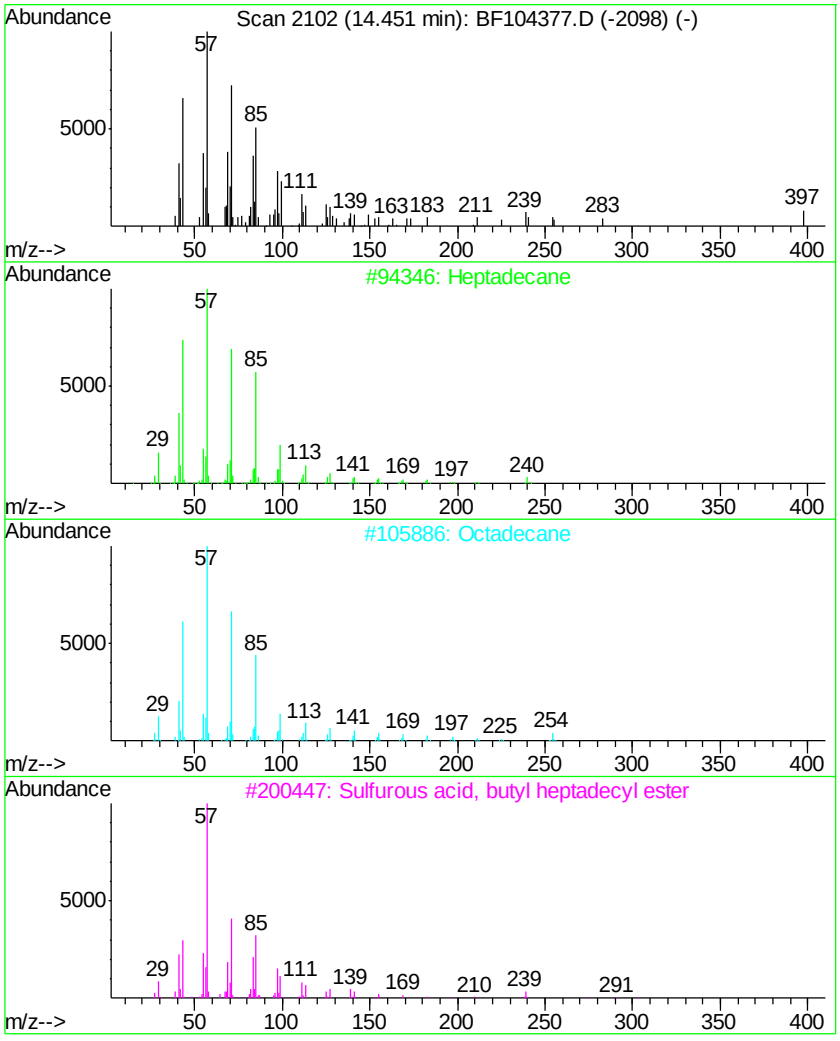
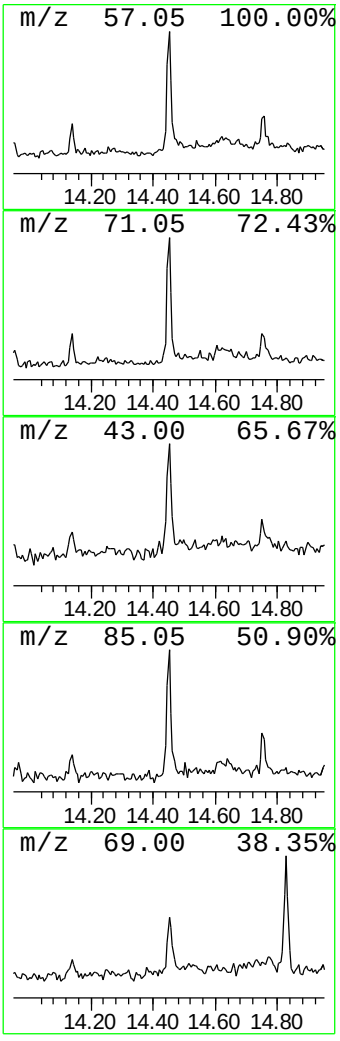
Peak Number 8 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.14 ng	84568	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Octadecane	254	C18H38	000593-45-3	92
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	87
4	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	86
5	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	74





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Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

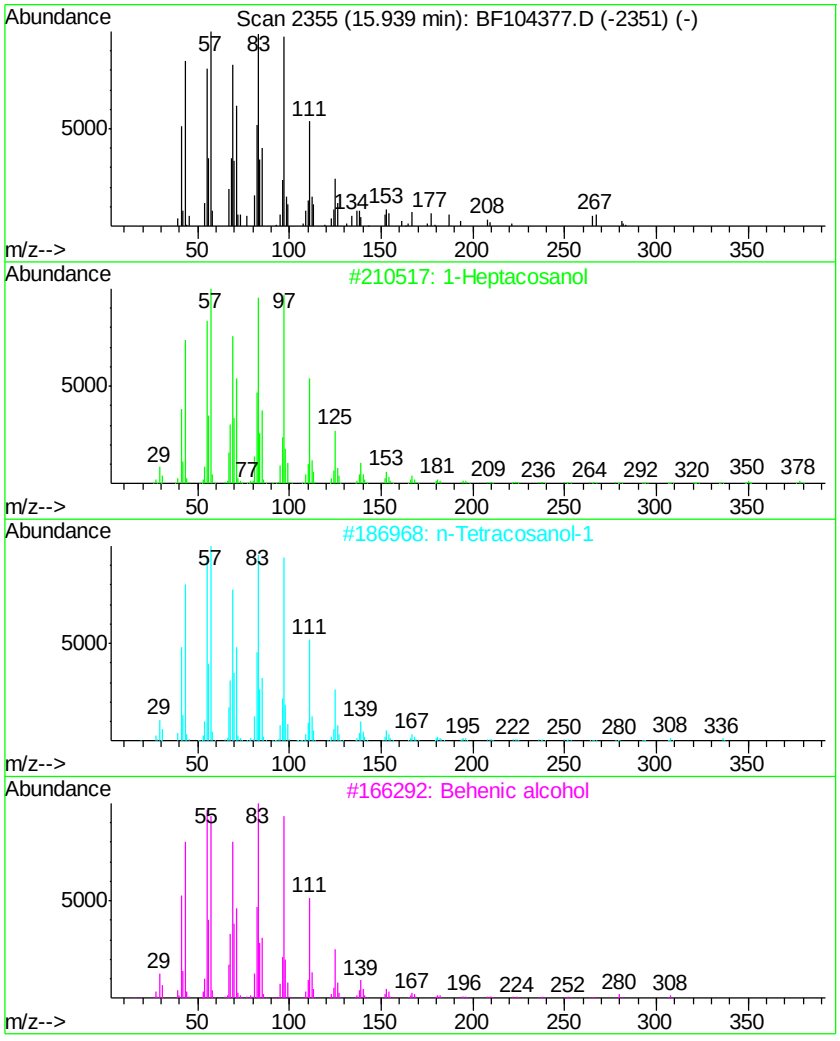
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

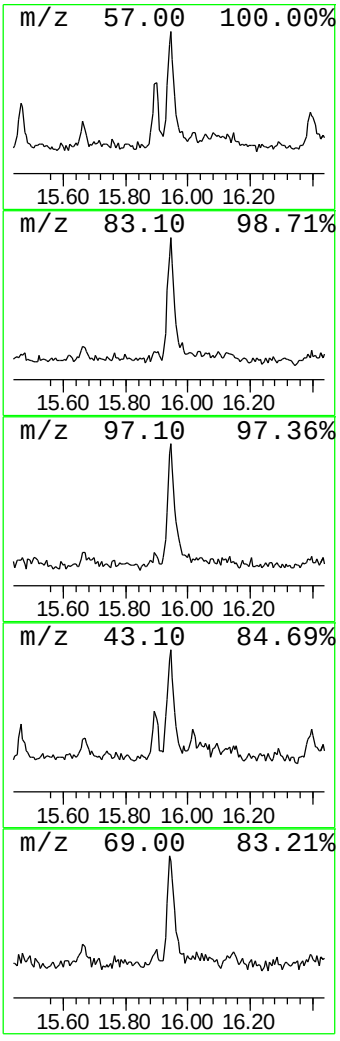
****

Peak Number 9 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.93 ng	121146	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104377.D
Acq On : 9 Apr 2018 17:30
Operator : JU/SJ
Sample : J2155-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.03	5.0	ng	207883	1	6.80	835094	20.0
Ethanol, 2-(2-met...	6.07	5.0	ng	210868	1	6.80	835094	20.0
unknown6.57	6.57	94.2	ng	3934890	1	6.80	835094	20.0
Hexadecane	10.75	2.3	ng	122776	4	11.33	1088460	20.0
n-Hexadecanoic acid	11.86	5.8	ng	317258	4	11.33	1088460	20.0
Behenic alcohol	13.81	12.1	ng	478257	5	13.97	790724	20.0
Heptadecane	14.45	2.1	ng	84568	5	13.97	790724	20.0
1-Heptacosanol	15.94	2.9	ng	121146	6	15.43	827198	20.0