LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

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-BF010918.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	4.934	480	484	496	rVB	198076	312460	7.53%	0.860%
2	5.340	547	553	556	rBV	3836807	4026552	96.98%	11.085%
3	6.369	721	728	732	rBV	3462465	4151928	100.00%	11.431%
4	6.492	744	749	752	rBV	3984842	4039896	97.30%	11.122%
5	6.722	784	788	791	rBV	986713	878864	21.17%	2.420%
6	6.875	810	814	818	rBV	3235400	3076432	74.10%	8.470%
7	7.287	878	884	887	rBV	2297593	2622735	63.17%	7.221%
8	7.998	1001	1005	1009	rBV	1237035	1143680	27.55%	3.149%
9	8.557	1096	1100	1104	rBV	448654	386896	9.32%	1.065%
10	9.081	1183	1189	1192	rBV	4093337	3817705	91.95%	10.510%
11	9.475	1251	1256	1259	rBV	1149718	919869	22.16%	2.532%
12	9.757	1299	1304	1307	rBV	1238980	1127216	27.15%	3.103%
13	10.475	1420	1426	1429	rBV	1907453	1840256	44.32%	5.066%
14	10.545	1433	1438	1441	rBV	2129799	2023383	48.73%	5.571%
15	11.239	1552	1556	1559	rVB	1074625	943884	22.73%	2.599%
16	12.821	1821	1825	1829	rBV	2457414	2451346	59.04%	6.749%
17	13.716	1973	1977	1981	rBV	400639	369157	8.89%	1.016%
18	13.874	1999	2004	2007	rBV	854795	782929	18.86%	2.155%
19	13.974	2016	2021	2025	rBV5	31617	41523	1.00%	0.114%
20	14.345	2080	2084	2089	rBV2	46441	61447	1.48%	0.169%
21	14.962	2185	2189	2196	rBV	65136	83772	2.02%	0.231%
22	15.292	2240	2245	2257	rBV	578589	804325	19.37%	2.214%
23	15.733	2315	2320	2323	rBV	58482	86193	2.08%	0.237%
24	15.774	2323	2327	2334	rVB2	52497	86631	2.09%	0.239%
25	16.209	2395	2401	2404	rBV2	53241	91401	2.20%	0.252%
26	16.756	2490	2494	2499	rVB2	38976	69264	1.67%	0.191%
27	17.415	2601	2606	2615	rVB3	37296	83118	2.00%	0.229%

Sum of corrected areas: 36322862

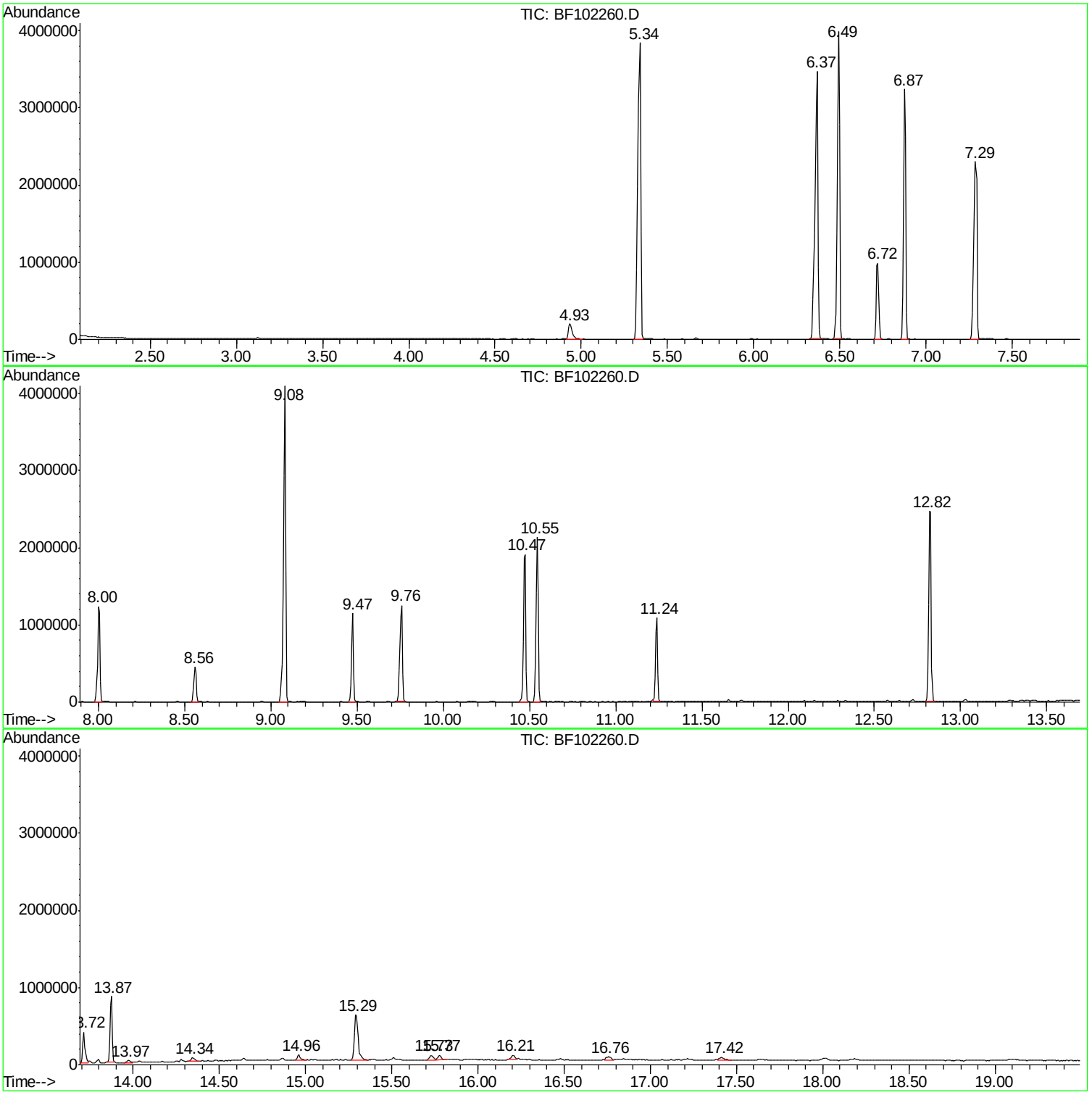
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

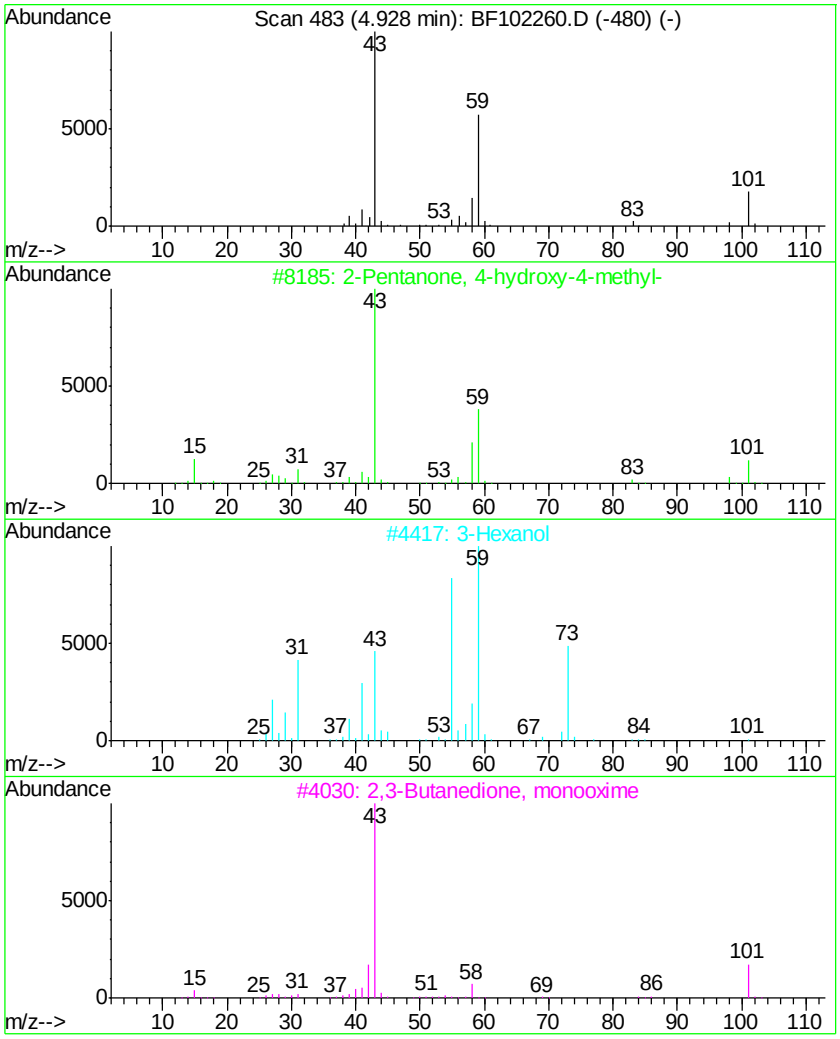
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

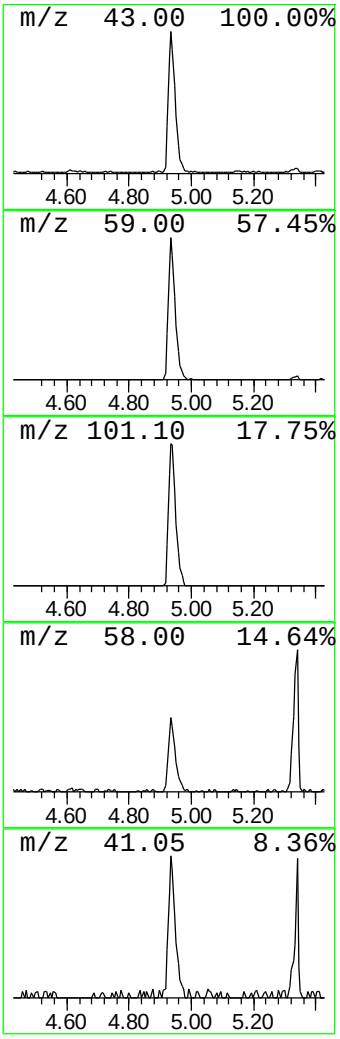
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	7.11 ng	312460	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

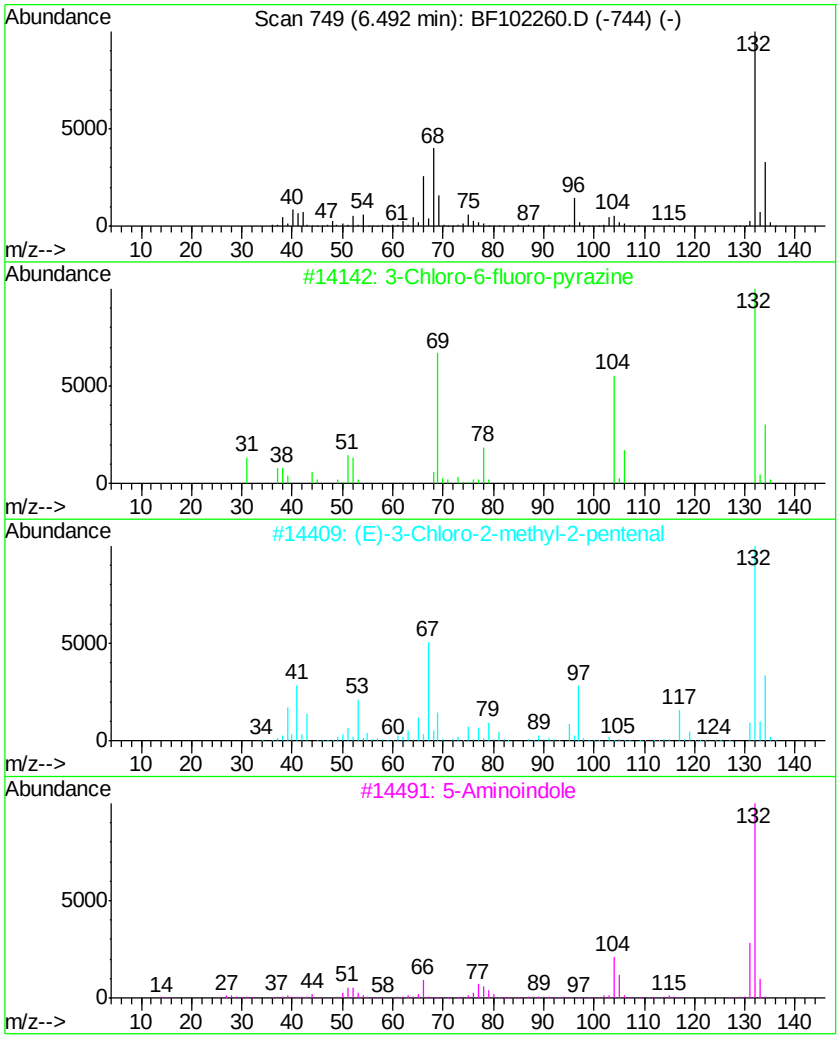
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

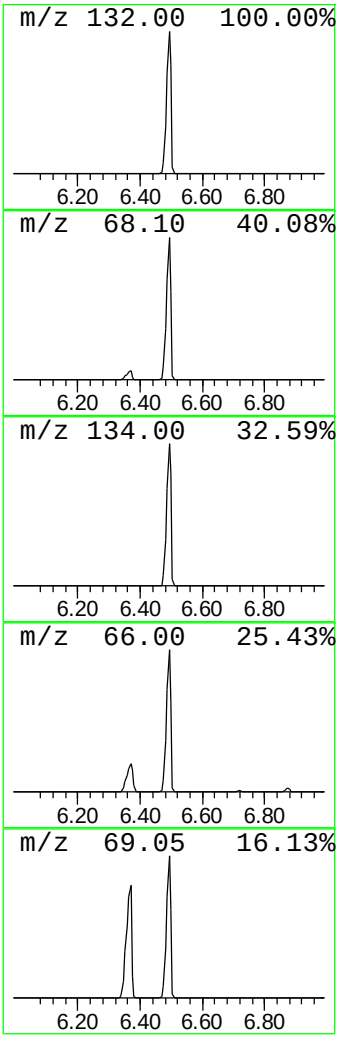
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	91.93 ng	4039900	1,4-Dichlorobenzene-d4	6.72

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	16
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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

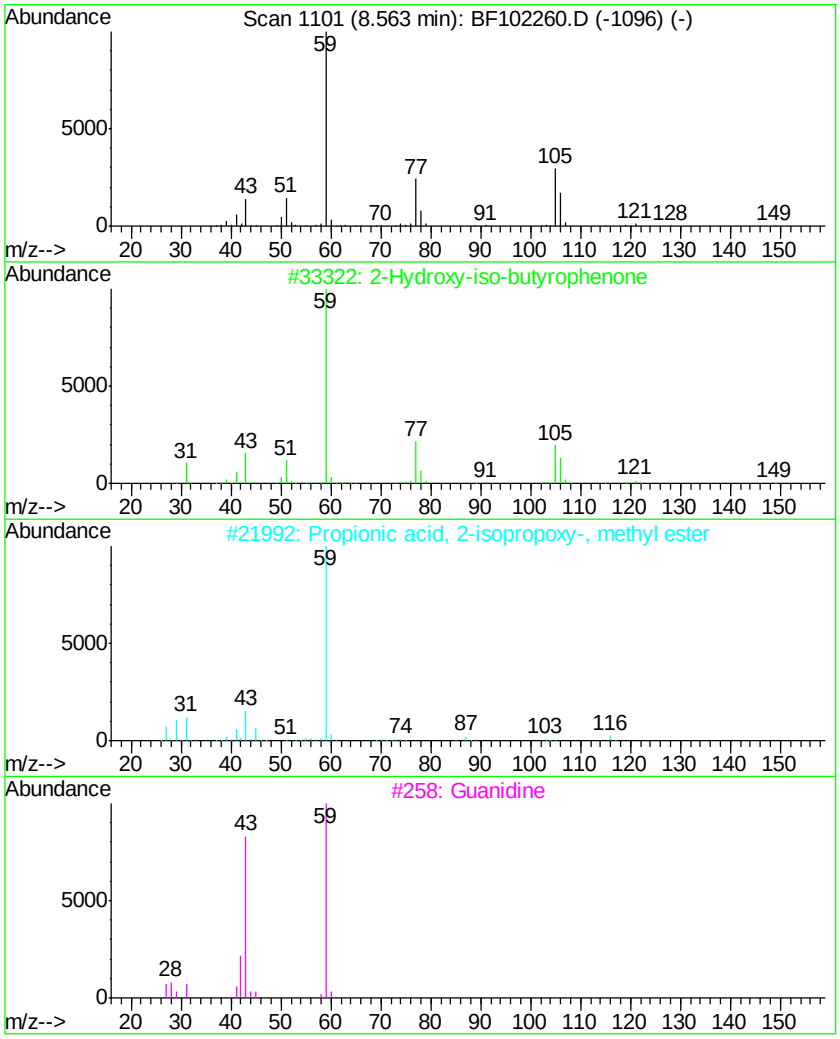
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

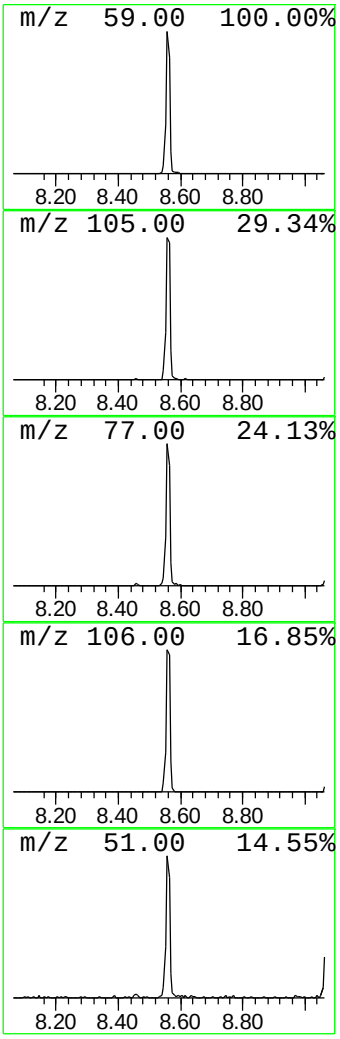
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	6.77 ng	386896	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
3	Guanidine	59	CH5N3	000113-00-8	7
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5	Acetamide	59	C2H5NO	000060-35-5	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

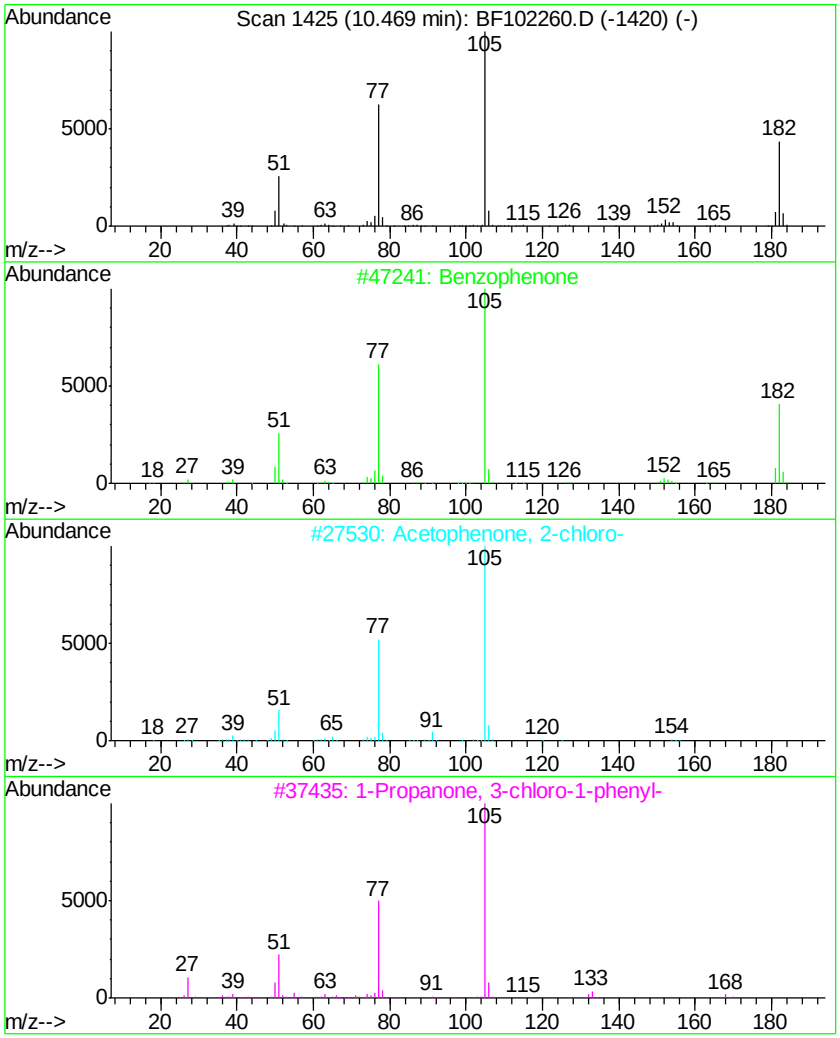
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

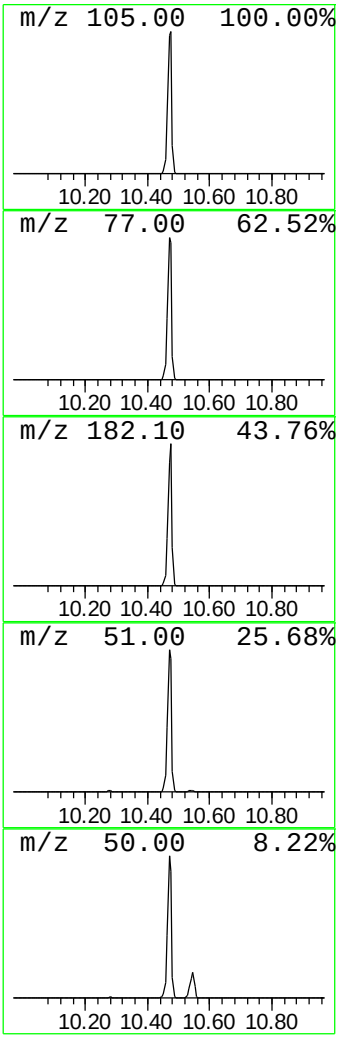
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	32.65 ng	1840260	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

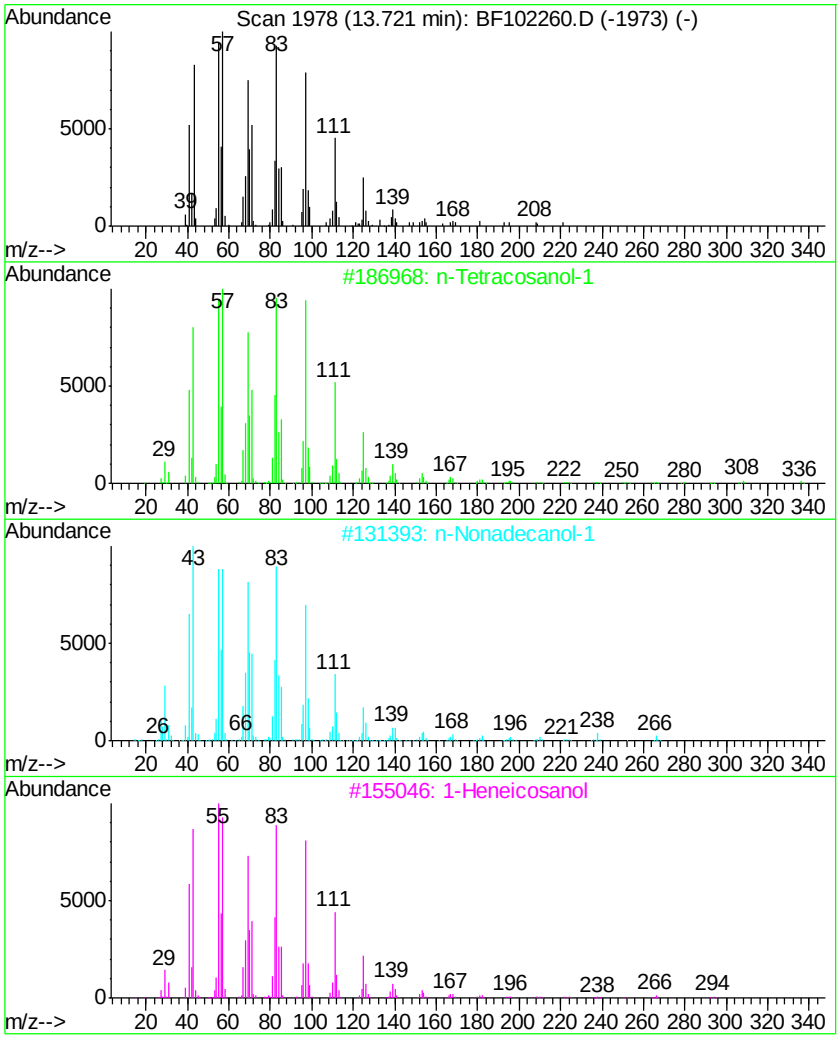
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

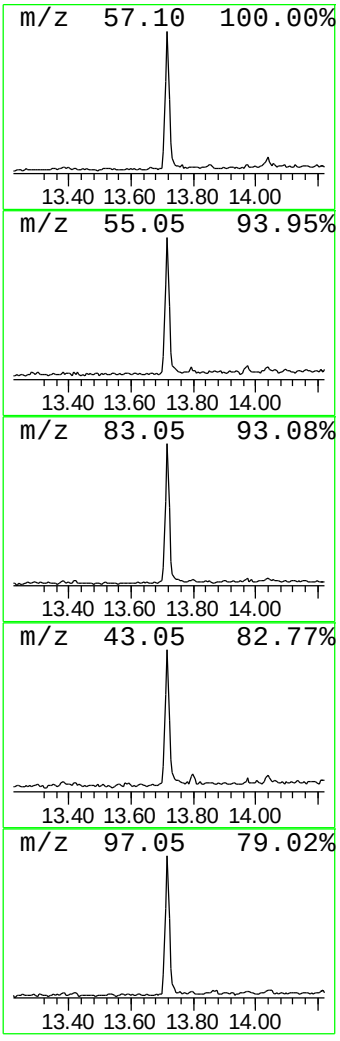
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	9.43 ng	369157	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Cycloeicosane	280	C20H40	000296-56-0	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

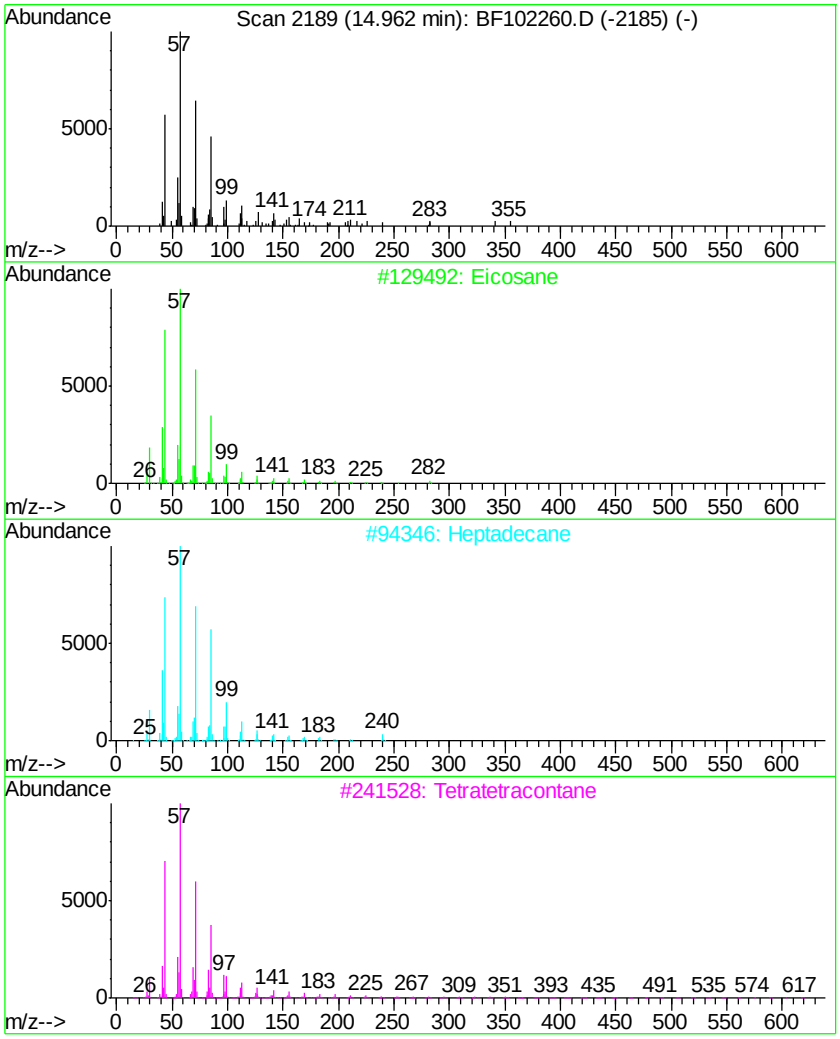
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

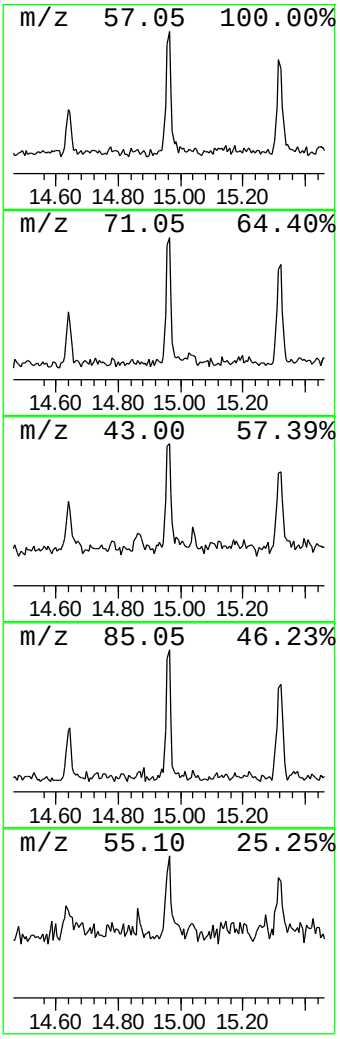
****

Peak Number 7 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.08 ng	83772	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heptadecane	240	C17H36	000629-78-7	87
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Hentriacontane	437	C31H64	000630-04-6	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

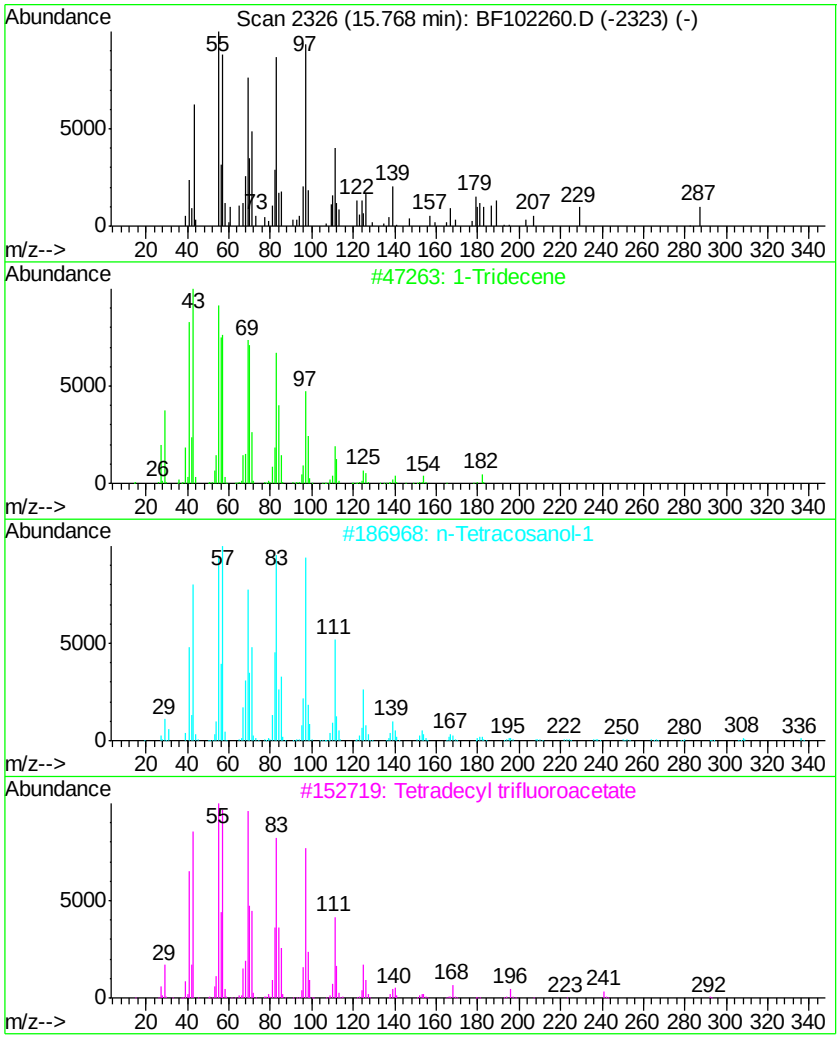
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

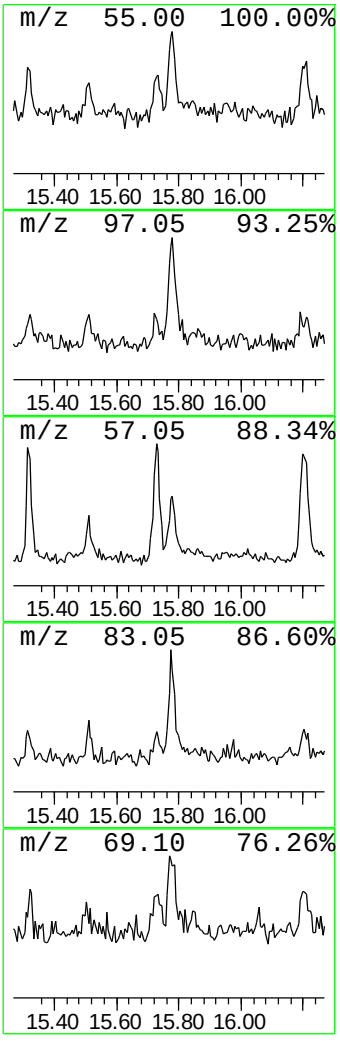
****

Peak Number 9 1-Tridecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.15 ng	86631	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecene	182	C13H26	002437-56-1	72
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	64
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	62
5	Behenic alcohol	326	C22H46O	000661-19-8	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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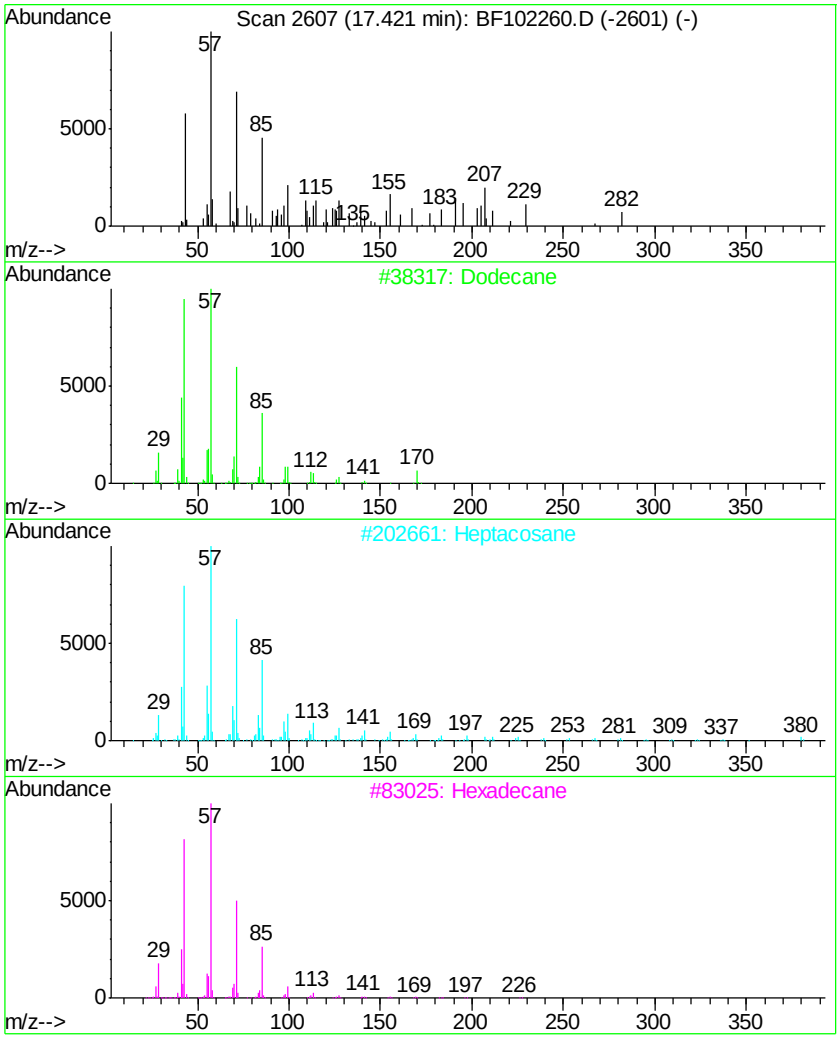
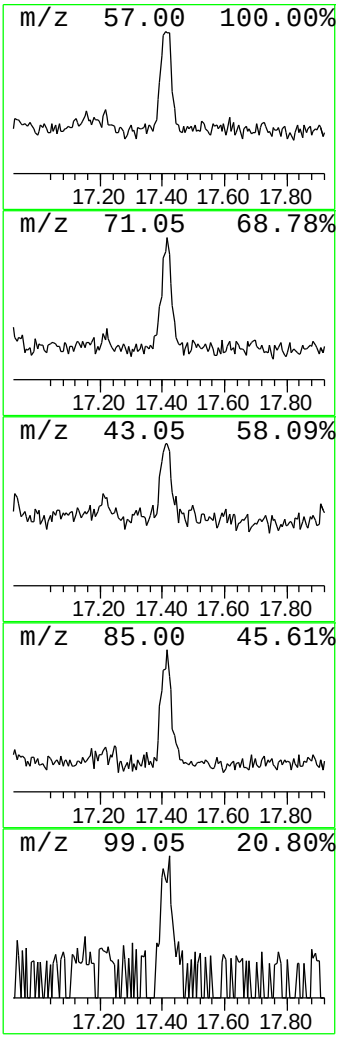
Peak Number 11 Dodecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	2.07 ng	83118	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	53
2	Heptacosane	380	C27H56	000593-49-7	50
3	Hexadecane	226	C16H34	000544-76-3	50
4	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	49
5	Hexacosane	366	C26H54	000630-01-3	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102260.D
Acq On : 20 Jan 2018 12:43
Operator : SJ/JU
Sample : J1115-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-32-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.93	7.1	ng	312460	1	6.72	878864	20.0
unknown6.49	6.49	91.9	ng	4039900	1	6.72	878864	20.0
2-Hydroxy-iso-but...	8.56	6.8	ng	386896	2	8.00	1143680	20.0
Benzophenone	10.47	32.6	ng	1840260	3	9.76	1127220	20.0
n-Tetracosanol-1	13.72	9.4	ng	369157	5	13.87	782929	20.0
Eicosane	14.96	2.1	ng	83772	6	15.30	804325	20.0
1-Tridecene	15.77	2.1	ng	86631	6	15.30	804325	20.0
Dodecane	17.42	2.1	ng	83118	6	15.30	804325	20.0