LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

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-BF072018.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	5.207	483	488	507	rBV	355806	573859	12.02%	1.469%
2	5.607	552	556	583	rBV	1999342	3527670	73.87%	9.032%
3	6.601	721	725	744	rBV	2241238	3514979	73.60%	9.000%
4	6.737	744	748	772	rVB	3061919	3830989	80.22%	9.809%
5	6.960	783	786	808	rVB	641587	904757	18.94%	2.317%
6	7.113	808	812	827	rBV	2661069	2942232	61.61%	7.533%
7	7.525	878	882	903	rBV	1719696	2384362	49.93%	6.105%
8	8.242	1000	1004	1019	rBV	1002531	1202264	25.17%	3.078%
9	9.313	1181	1186	1208	rBV	3840441	4597101	96.26%	11.770%
10	9.948	1287	1294	1298	rBV2	56914	127327	2.67%	0.326%
11	10.001	1298	1303	1316	rVB2	1305181	1377697	28.85%	3.527%
12	10.795	1434	1438	1463	rBV	2526941	3196138	66.92%	8.183%
13	11.495	1553	1557	1579	rBV	1341588	1560301	32.67%	3.995%
14	12.001	1639	1643	1647	rBV2	38470	59303	1.24%	0.152%
15	13.083	1822	1827	1841	rBV	4328563	4775824	100.00%	12.228%
16	14.148	2004	2008	2022	rBV	1051206	1240654	25.98%	3.177%
17	14.271	2026	2029	2035	rBV2	44900	54328	1.14%	0.139%
18	14.583	2078	2082	2087	rVB	137948	145537	3.05%	0.373%
19	14.901	2131	2136	2141	rBV	297156	342503	7.17%	0.877%
20	15.254	2192	2196	2204	rVB	403350	490256	10.27%	1.255%
21	15.677	2259	2268	2279	rBV2	695084	1597474	33.45%	4.090%
22	16.118	2338	2343	2348	rVB	250393	395397	8.28%	1.012%
23	16.654	2429	2434	2440	rVB	120338	215471	4.51%	0.552%

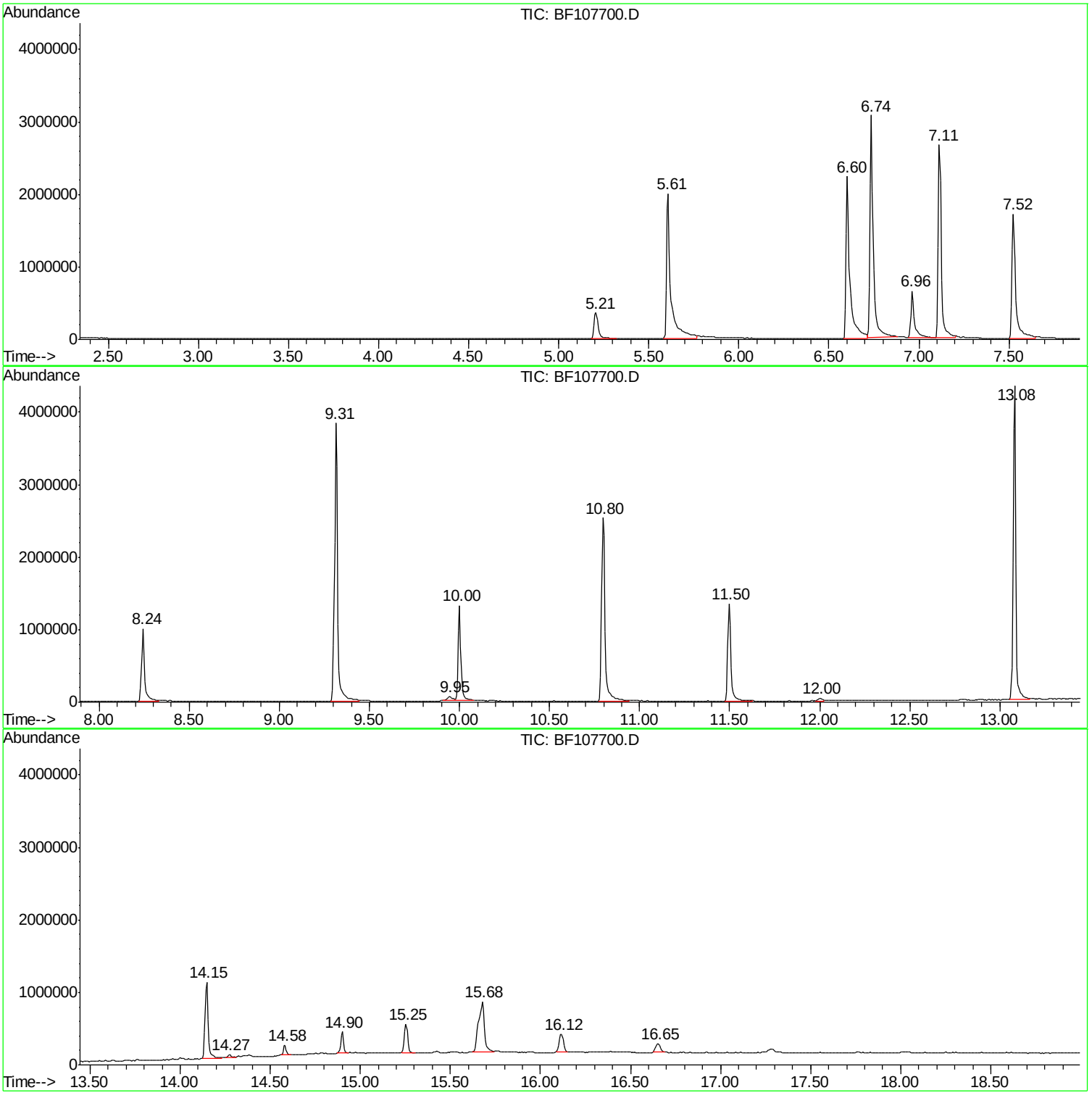
Sum of corrected areas: 39056423

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

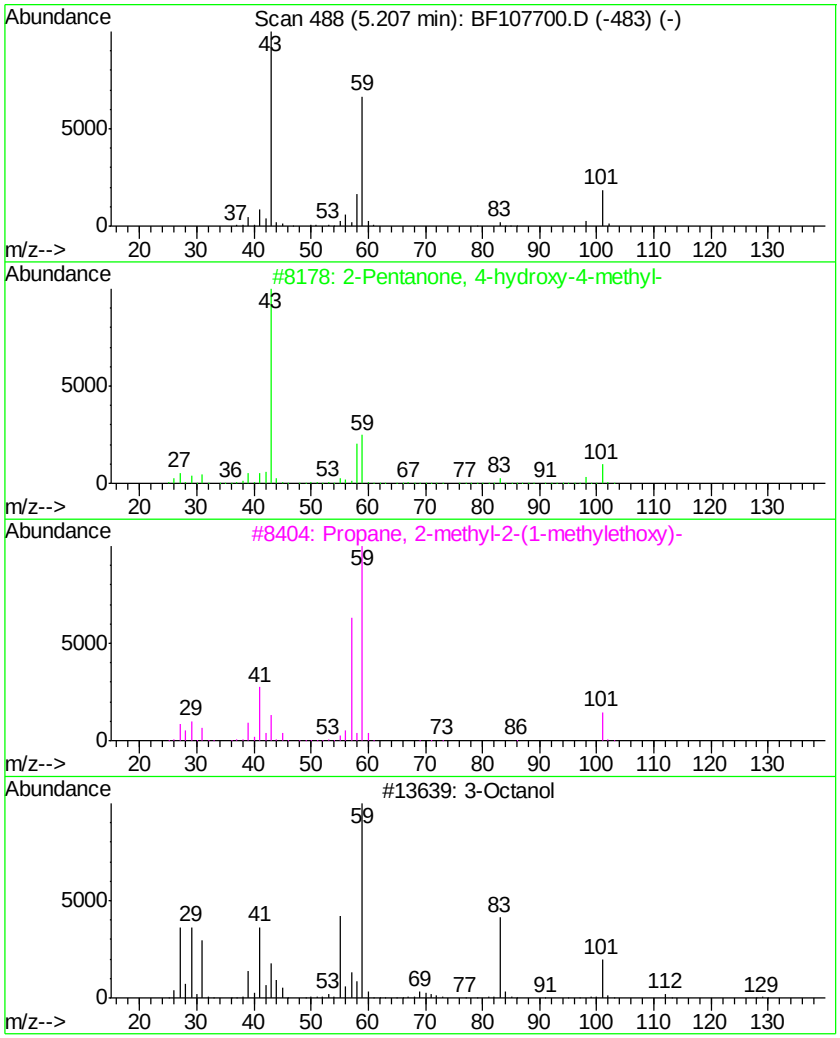
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

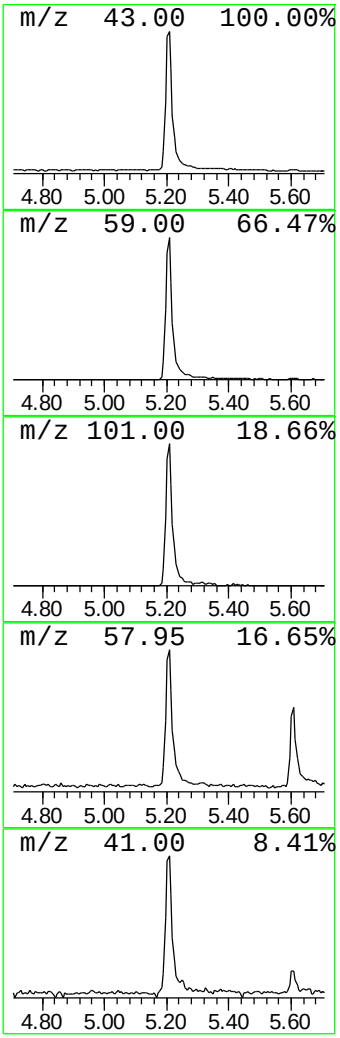
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	12.69 ng	573859	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	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Octanol	130	C8H18O	000589-98-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

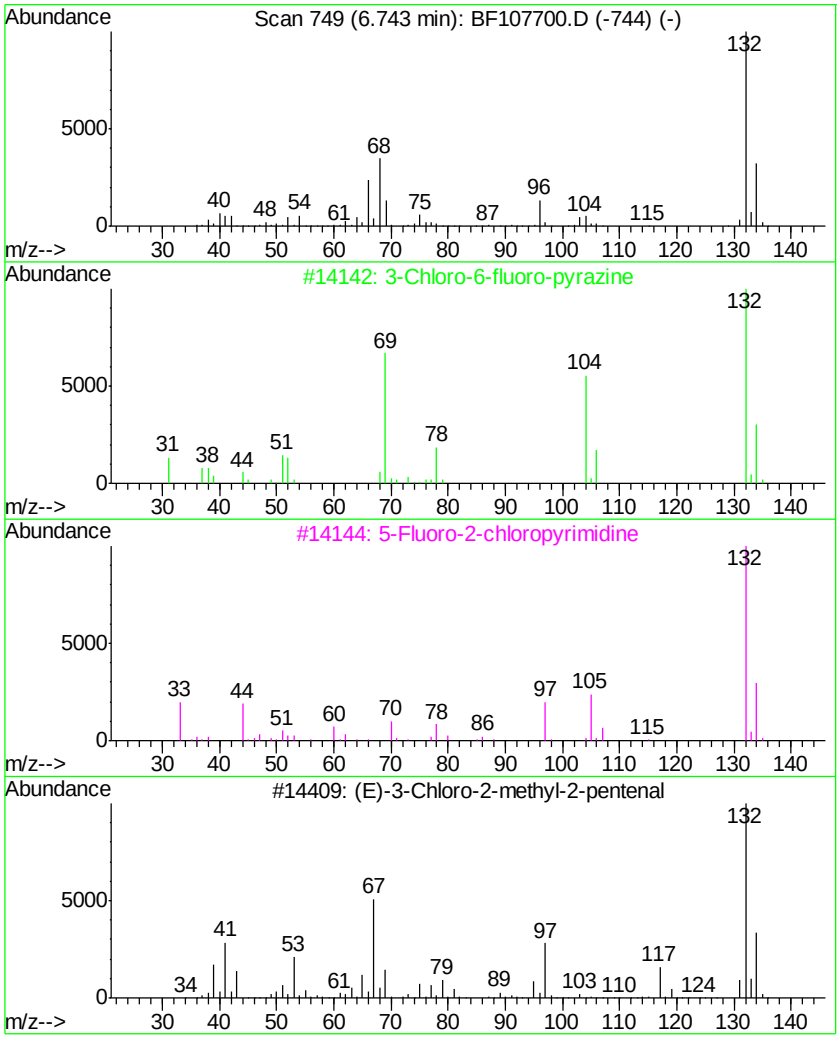
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

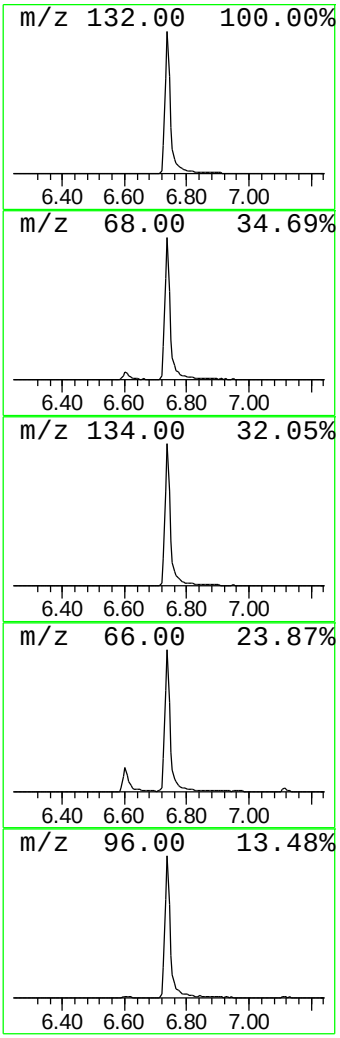
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	84.69 ng	3830990	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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

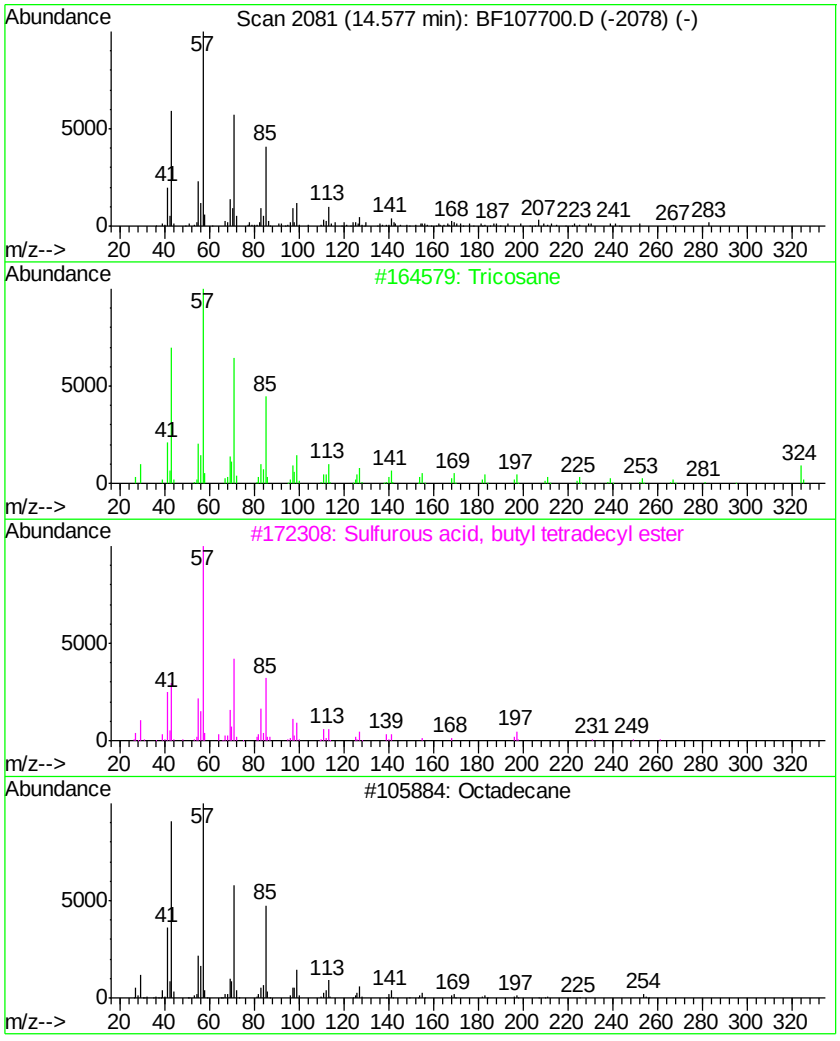
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

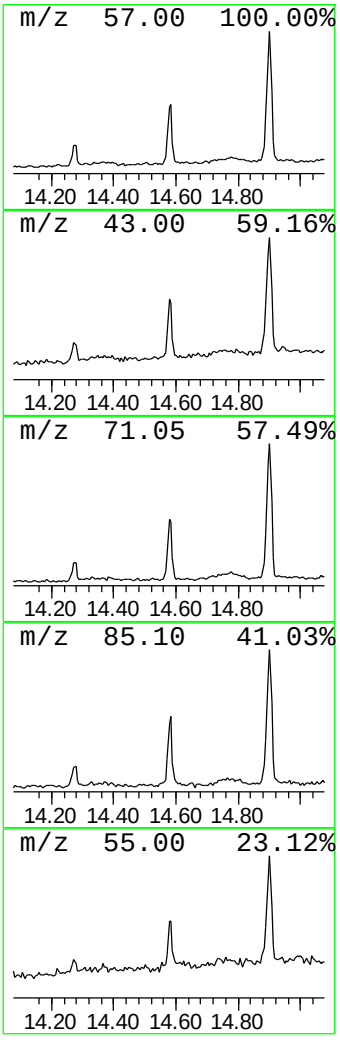
****

Peak Number 4 Sulfurous acid, butyl tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.35 ng	145537	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
3	Octadecane	254	C18H38	000593-45-3	80
4	Docosane	310	C22H46	000629-97-0	78
5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

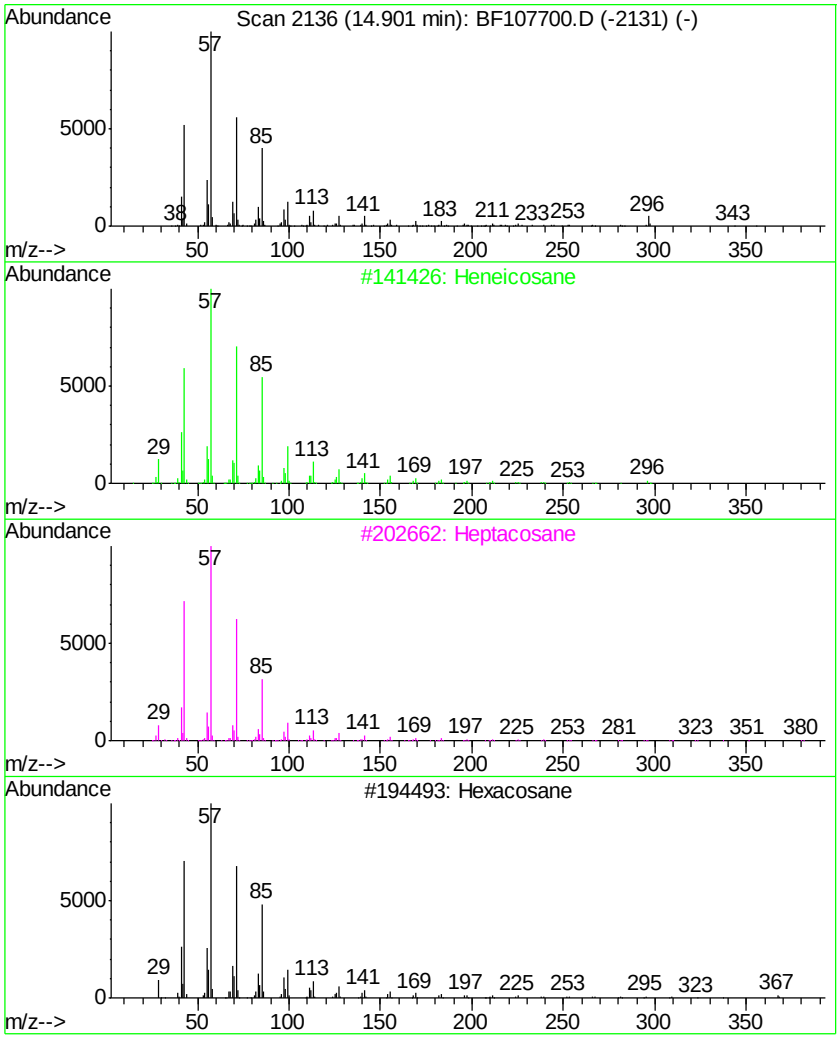
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

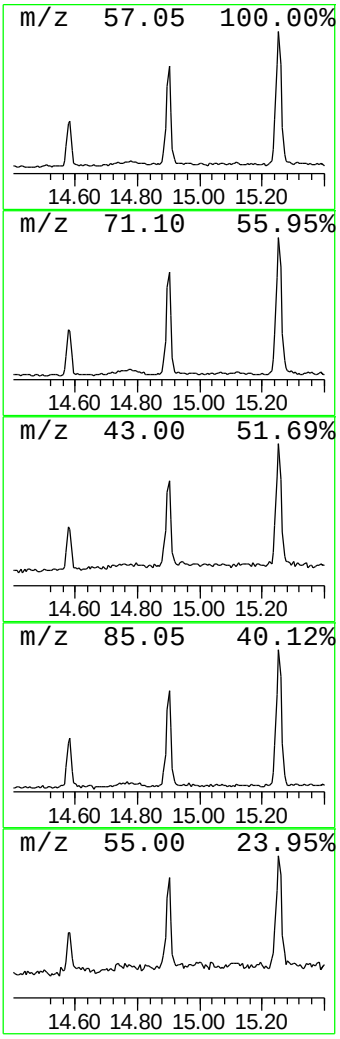
****

Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	5.52 ng	342503	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptacosane	380	C27H56	000593-49-7	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

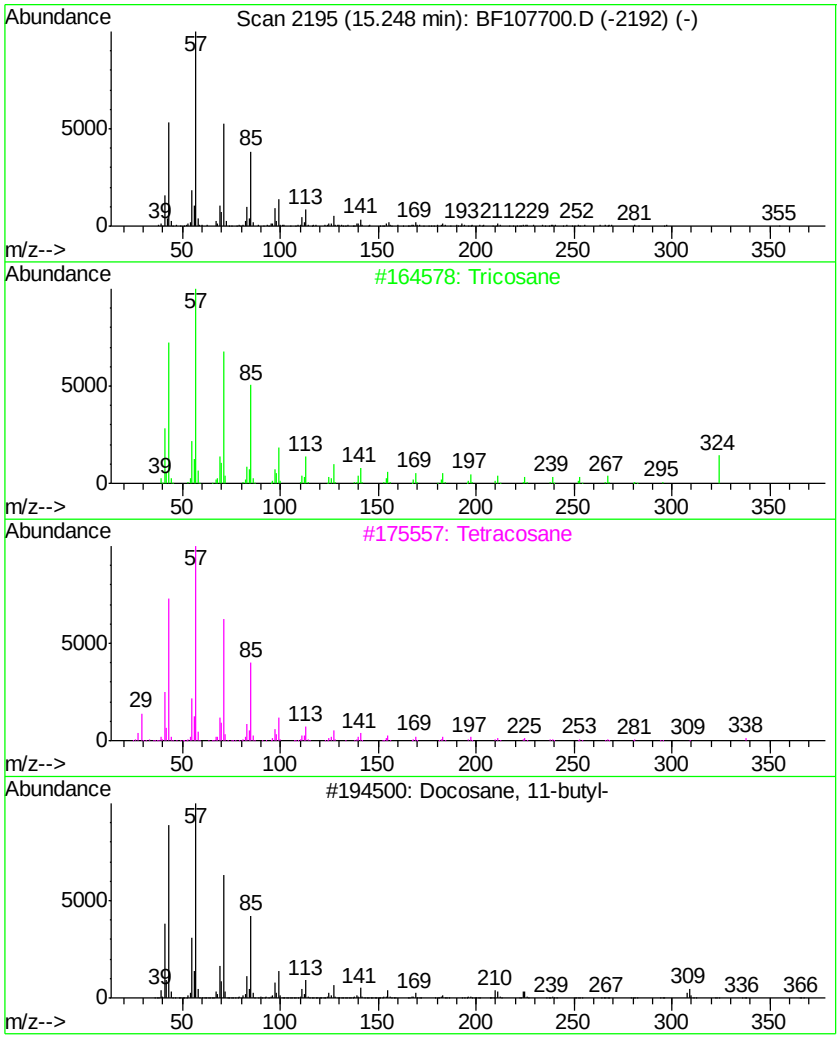
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

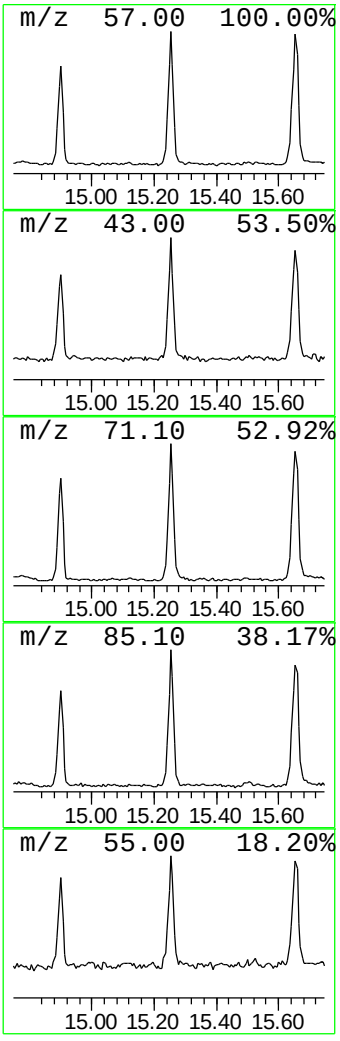
****

Peak Number 6 Tricosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	6.14 ng	490256	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Tetracosane	338	C24H50	000646-31-1	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

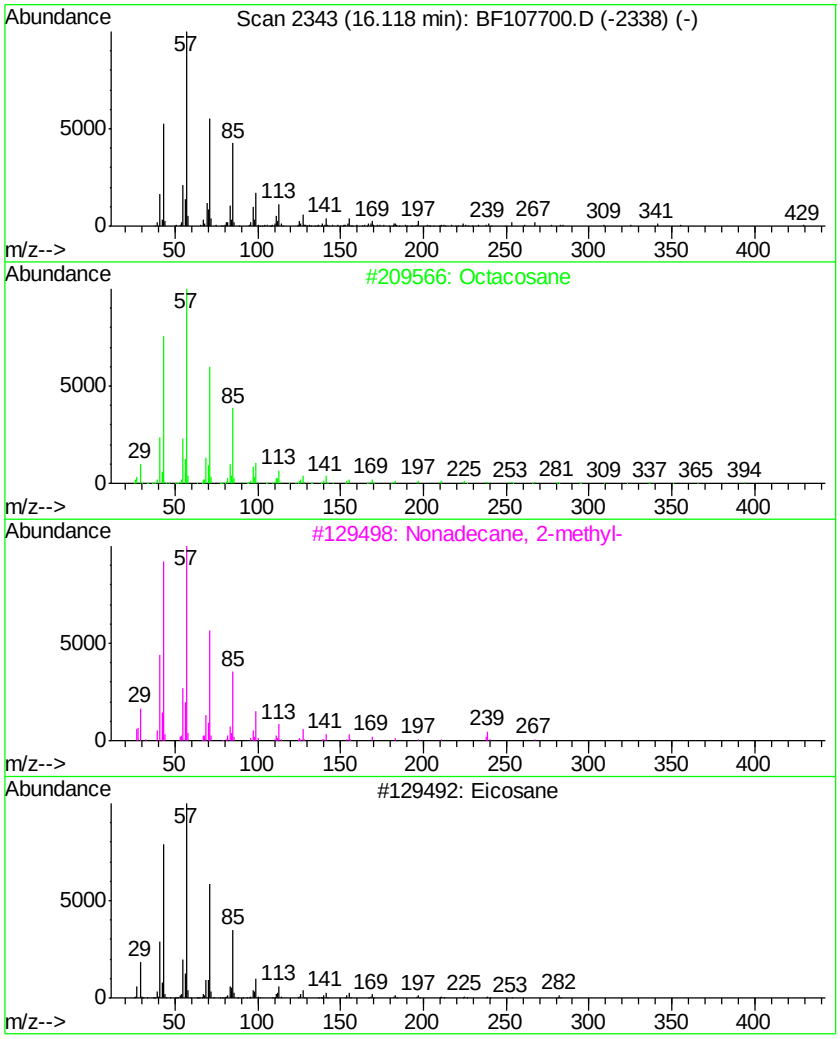
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

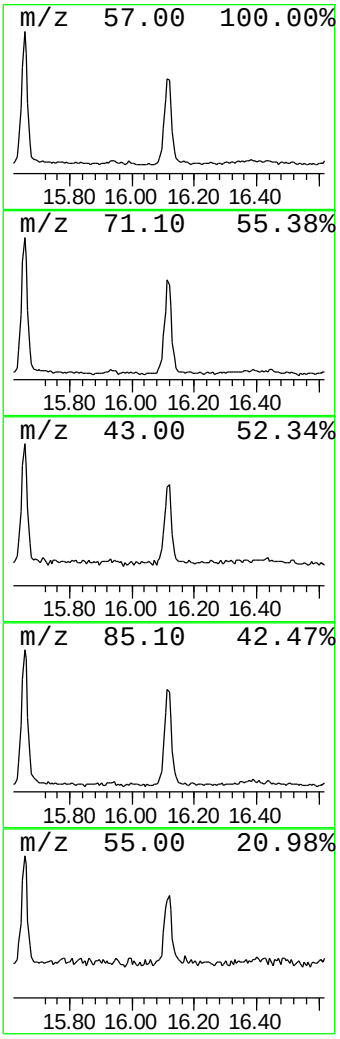
****

Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	4.95 ng	395397	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
3	Eicosane	282	C20H42	000112-95-8	86
4	Docosane	310	C22H46	000629-97-0	86
5	2-methyloctacosane	408	C29H60	1000376-72-8	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

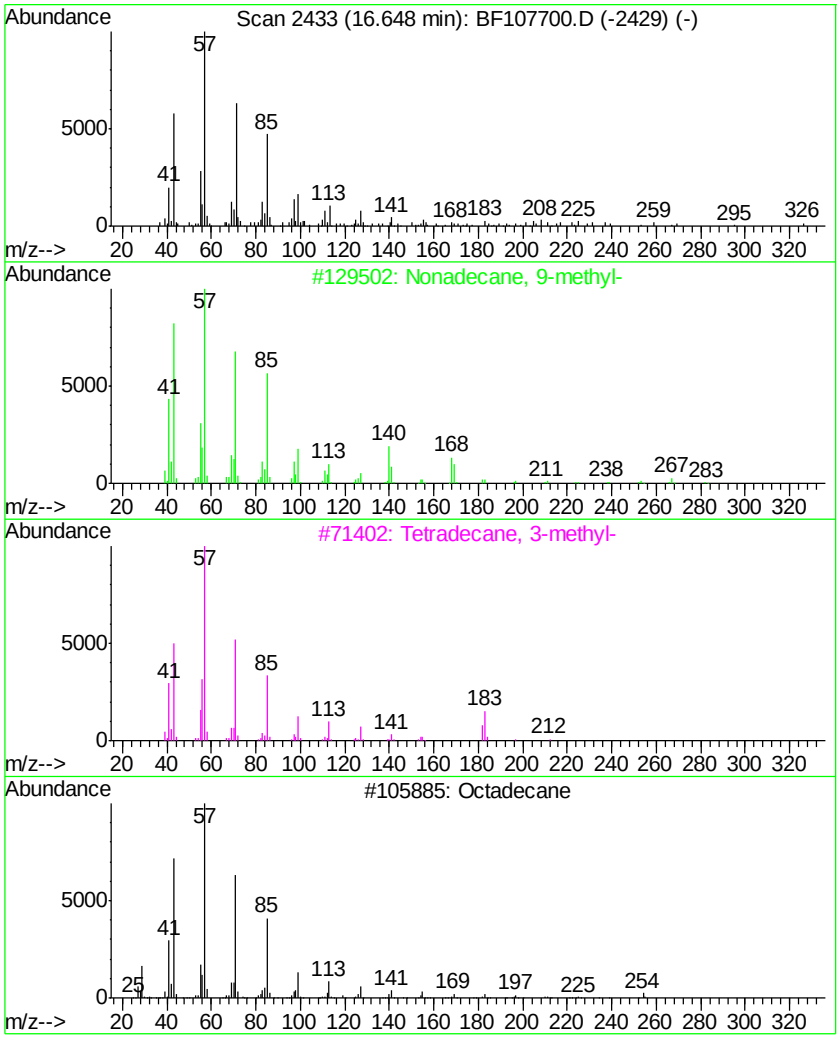
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

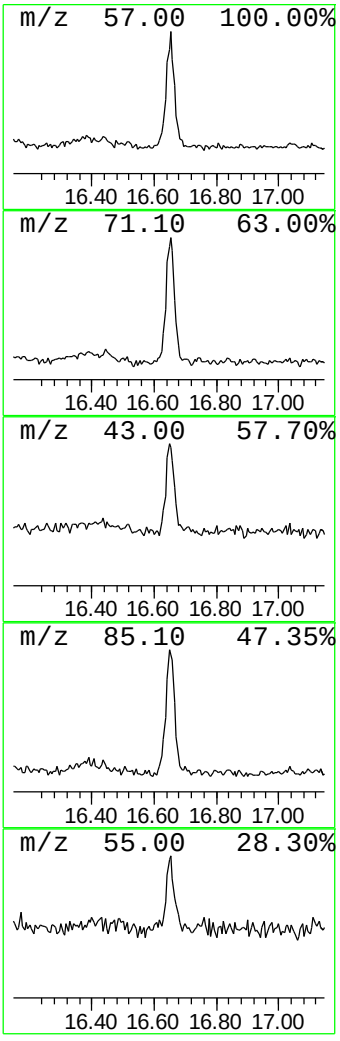
****

Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	2.70 ng	215471	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
2	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	87
3	Octadecane	254	C18H38	000593-45-3	83
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5	Eicosane	282	C20H42	000112-95-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107700.D
Acq On : 26 Jul 2018 15:30
Operator : JU/SJ
Sample : PB111479BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB111479BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.21	12.7	ng	573859	1	6.96	904757	20.0
unknown6.74	6.74	84.7	ng	3830990	1	6.96	904757	20.0
Sulfurous acid, b...	14.58	2.4	ng	145537	5	14.15	1240650	20.0
Heneicosane	14.90	5.5	ng	342503	5	14.15	1240650	20.0
Tricosane	15.25	6.1	ng	490256	6	15.68	1597470	20.0
Octacosane	16.12	5.0	ng	395397	6	15.68	1597470	20.0
Nonadecane, 9-met...	16.65	2.7	ng	215471	6	15.68	1597470	20.0