LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

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-BF092218.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	4.904	475	479	487	rBV	54466	75411	2.82%	0.340%
2	5.316	544	549	552	rBV	2045249	2010581	75.12%	9.076%
3	6.339	718	723	726	rBV	2062547	2102195	78.54%	9.489%
4	6.475	741	746	749	rBV	2243290	2116029	79.06%	9.552%
5	6.704	781	785	788	rBV	736116	576437	21.54%	2.602%
6	6.863	807	812	815	rBV	1979013	1674773	62.57%	7.560%
7	7.263	875	880	883	rBV	1460416	1328261	49.63%	5.996%
8	7.986	999	1003	1006	rBV	889885	739905	27.64%	3.340%
9	9.063	1180	1186	1189	rBV	2984592	2516171	94.01%	11.358%
10	9.733	1296	1300	1304	rBV	1050521	845058	31.57%	3.814%
11	10.516	1429	1433	1449	rBV	1479128	1285590	48.03%	5.803%
12	11.210	1547	1551	1554	rBV	1102966	902005	33.70%	4.072%
13	12.792	1815	1820	1823	rBV	2830862	2676560	100.00%	12.082%
14	13.833	1993	1997	2000	rBV	954561	816188	30.49%	3.684%
15	14.321	2077	2080	2085	rVB	68133	63203	2.36%	0.285%
16	14.615	2122	2130	2135	rBV	190923	208084	7.77%	0.939%
17	14.933	2177	2184	2193	rBV	366478	415411	15.52%	1.875%
18	15.227	2230	2234	2239	rBV	501977	577822	21.59%	2.608%
19	15.286	2239	2244	2256	rVB	422113	523934	19.57%	2.365%
20	15.686	2304	2312	2323	rBV	275633	424799	15.87%	1.917%
21	16.145	2381	2390	2398	rBV	115555	210289	7.86%	0.949%
22	16.686	2471	2482	2491	rBV2	30168	65173	2.43%	0.294%

Sum of corrected areas: 22153879

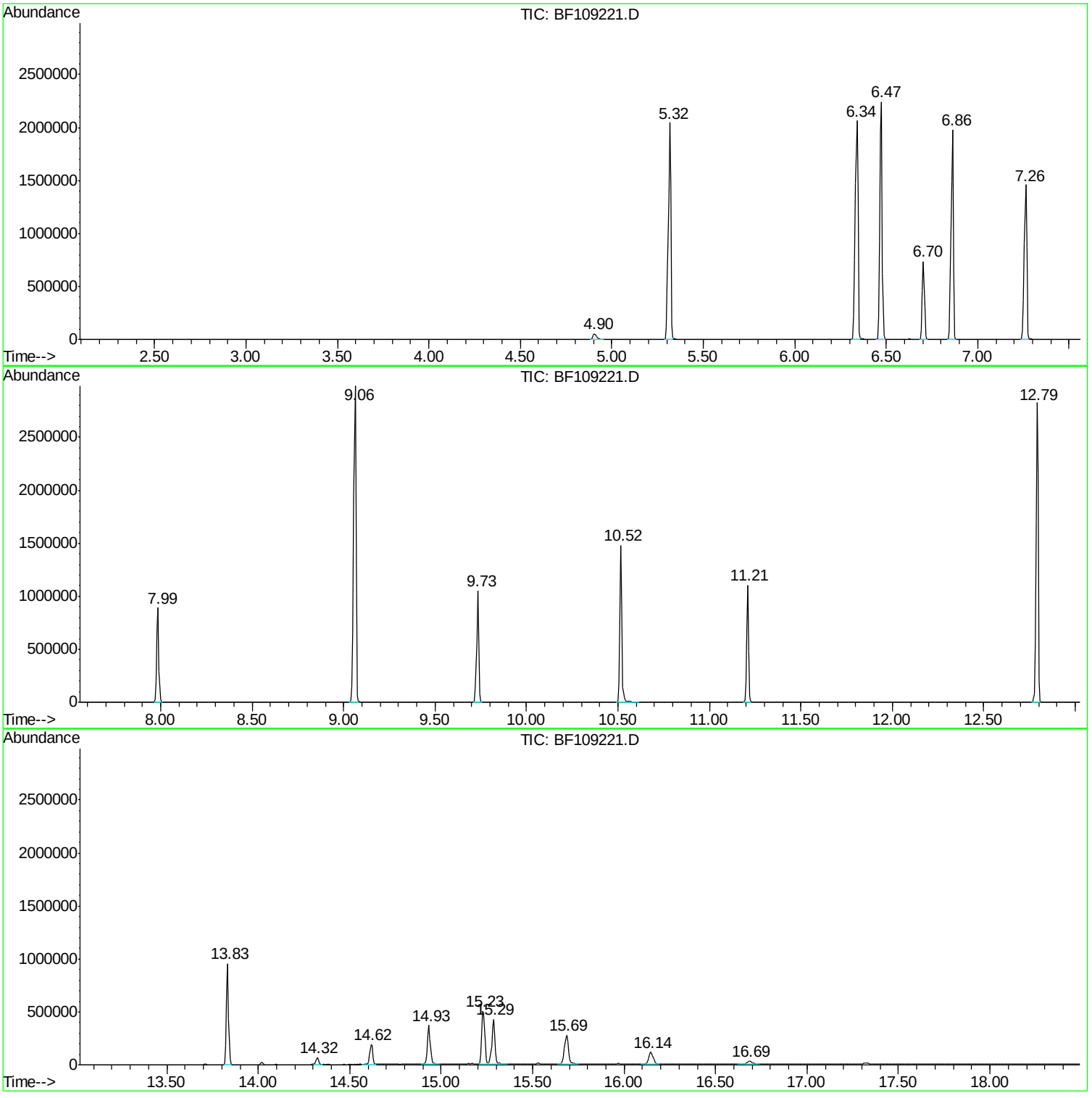
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

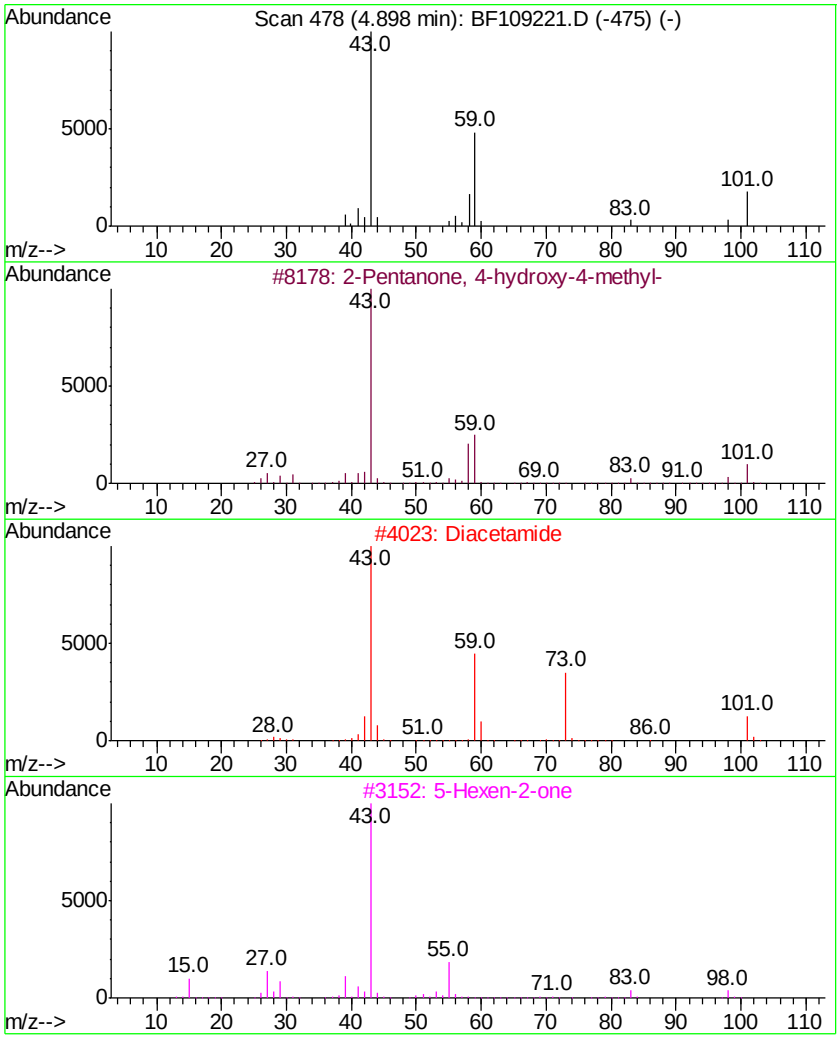
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

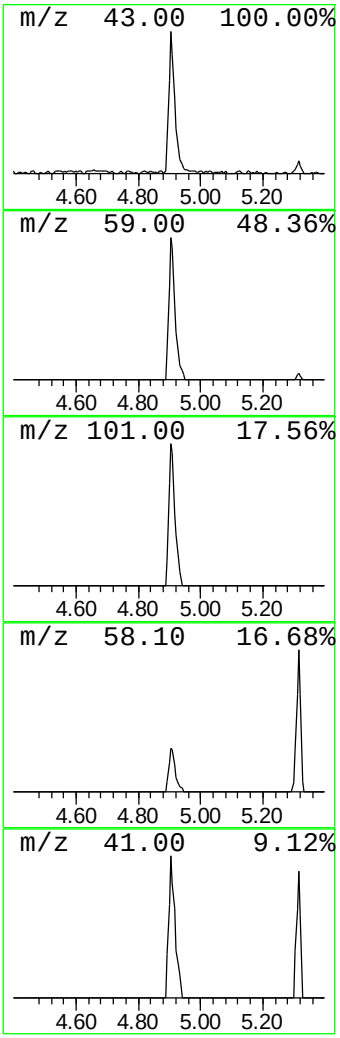
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.62 ng	75411	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Diacetamide	101	C4H7NO2	000625-77-4	36
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

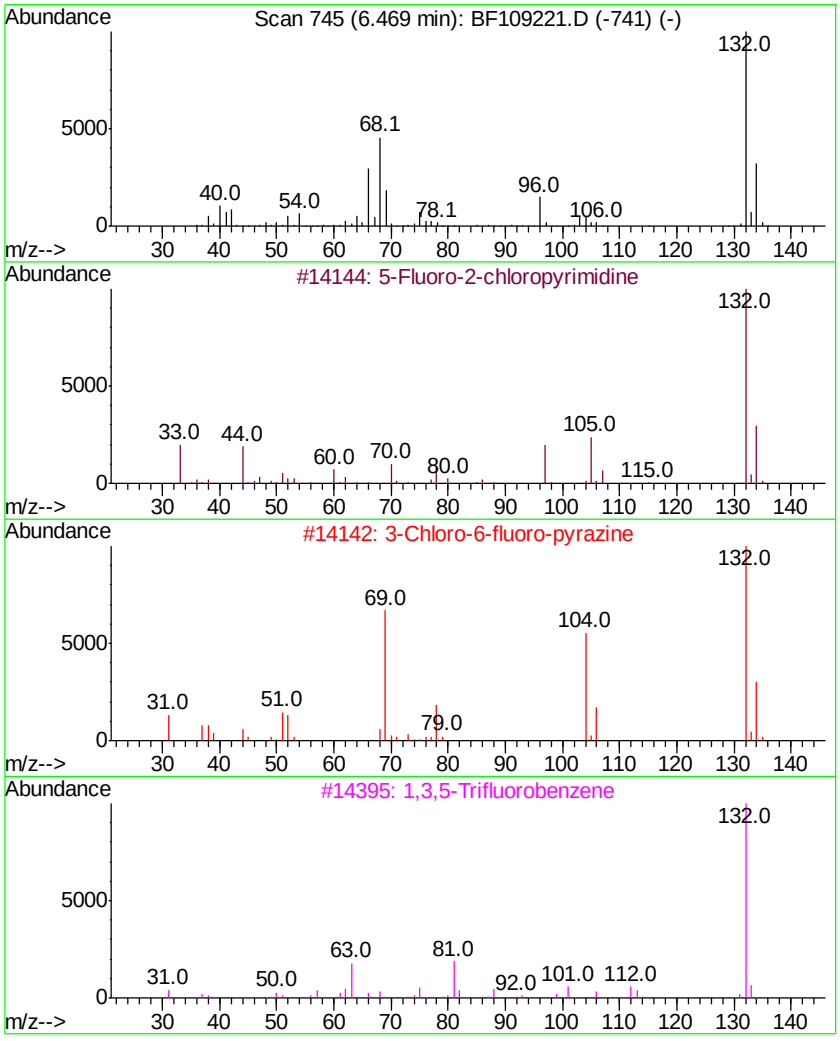
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

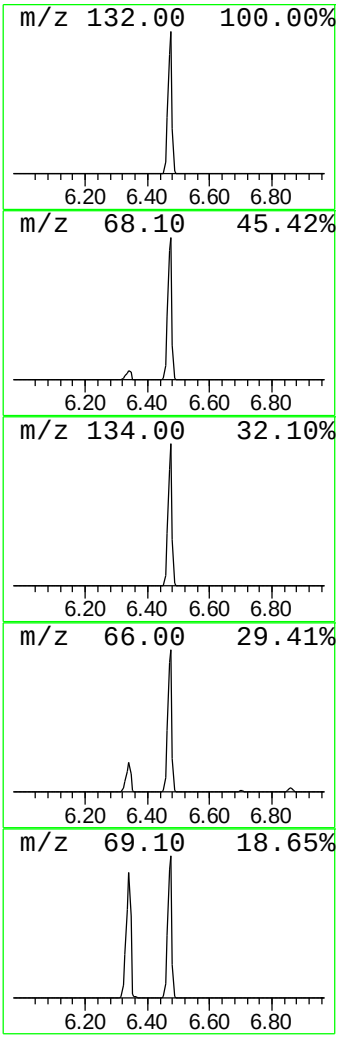
****

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	73.42 ng	2116030	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

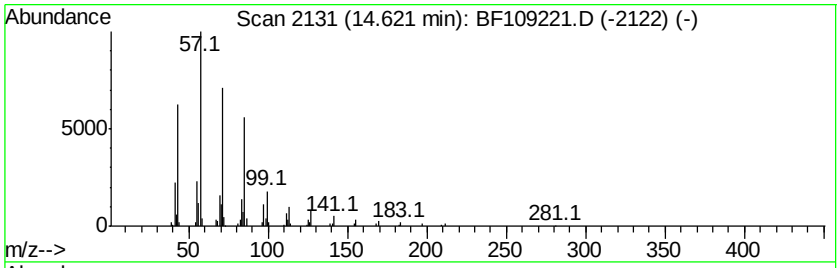
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

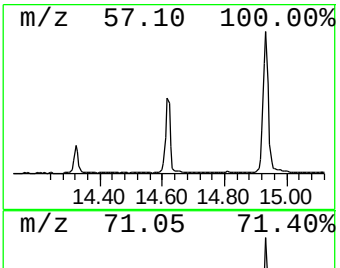
****

Peak Number 4 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	7.20 ng	208084	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptadecane	240	C17H36	000629-78-7	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

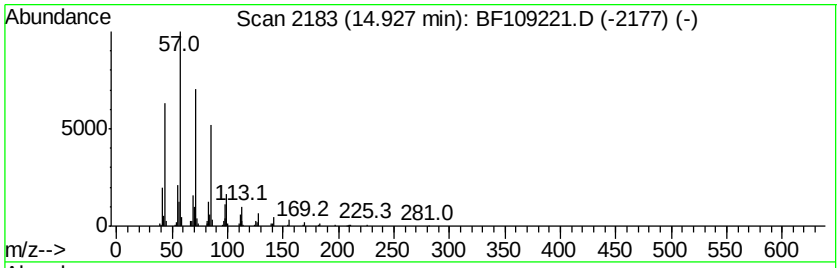
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

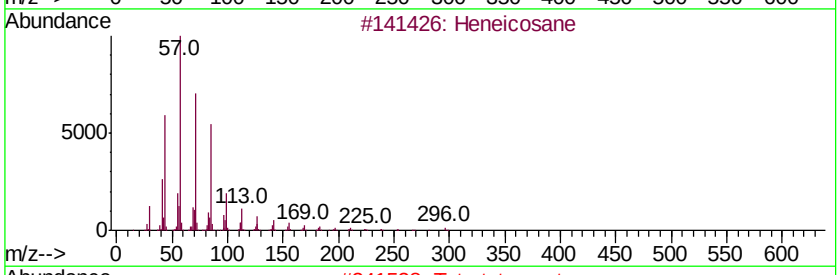
****

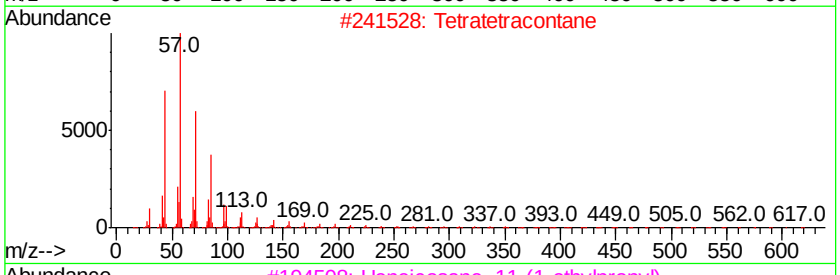
Peak Number 5 Heneicosane Concentration Rank 5

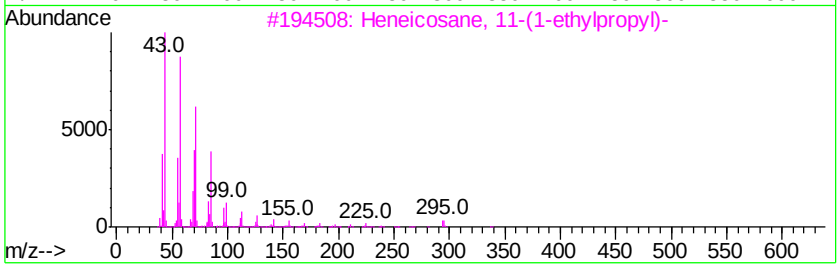
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	14.38 ng	415411	Perylene-d12	15.23

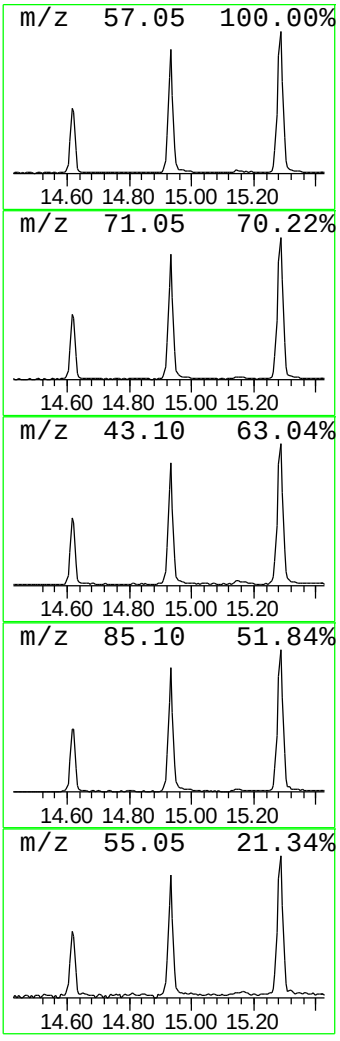
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87











Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

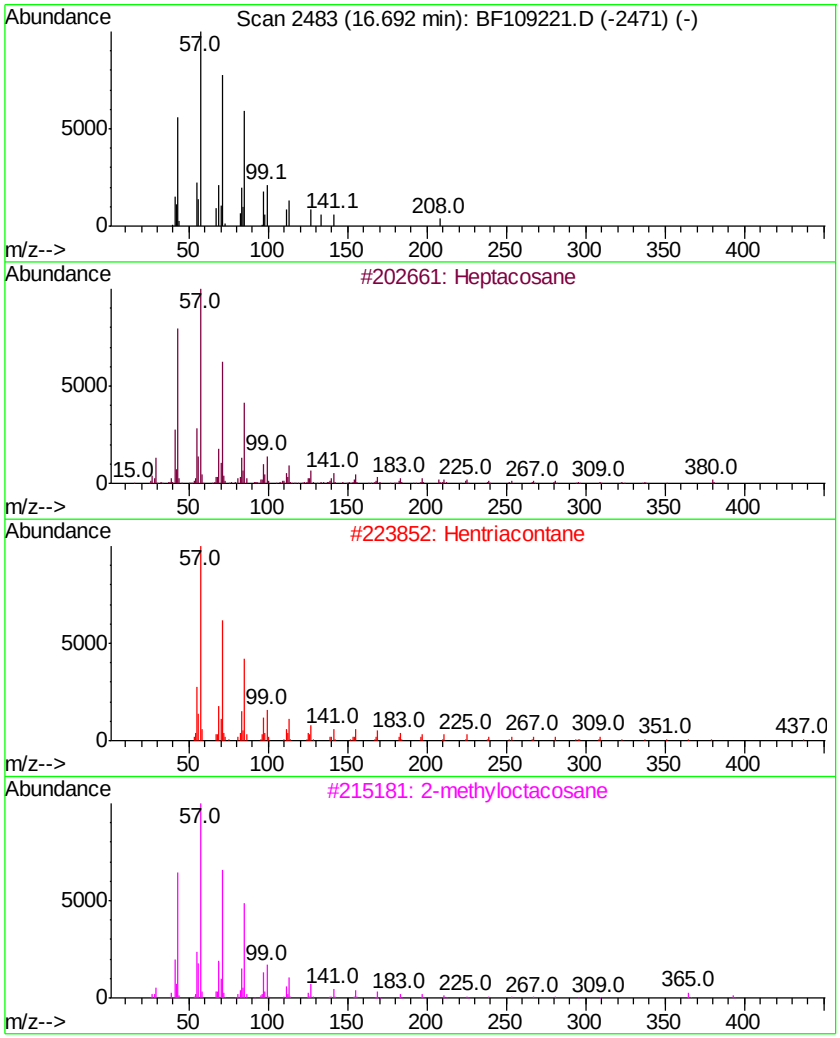
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

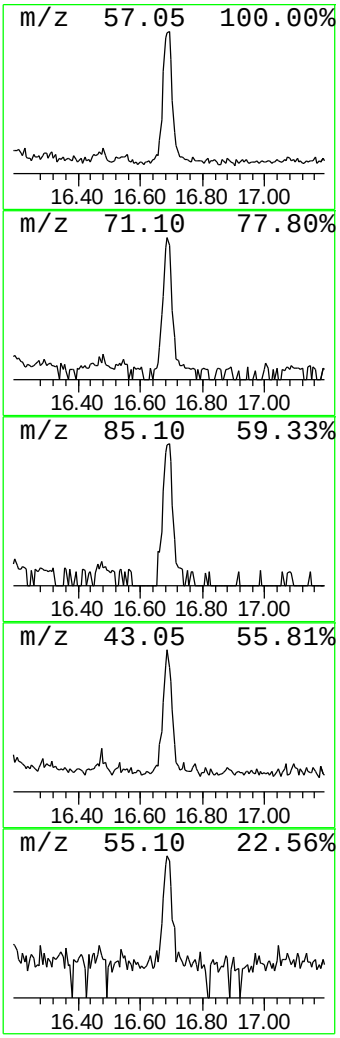
****

Peak Number 9 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	2.26 ng	65173	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	2-methyltetracosane	352	C25H52	1000376-72-6	90
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092218\
Data File : BF109221.D
Acq On : 22 Sep 2018 15:14
Operator : JU/SJ
Sample : PB113095BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB113095BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.90	2.6	ng	75411	1	6.70	576437	20.0
unknown6.47	6.47	73.4	ng	2116030	1	6.70	576437	20.0
Octacosane	14.62	7.2	ng	208084	6	15.23	577822	20.0
Heneicosane	14.93	14.4	ng	415411	6	15.23	577822	20.0
Heptacosane	16.69	2.3	ng	65173	6	15.23	577822	20.0