LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113237.D
Acq On : 22 Mar 2019 16:25
Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	5.334	547	552	555	rBV	3388519	3478358	89.90%	9.648%
2	6.363	722	727	730	rBV	3103510	3463595	89.52%	9.607%
3	6.487	744	748	752	rBV	3833426	3869160	100.00%	10.732%
4	6.710	783	786	790	rBV	925564	872818	22.56%	2.421%
5	6.869	809	813	817	rBV	2965032	2827869	73.09%	7.844%
6	7.275	877	882	885	rBV	2177283	2300257	59.45%	6.380%
7	7.998	1000	1005	1011	rBV	1132815	1181876	30.55%	3.278%
8	9.075	1183	1188	1191	rBV	4096888	3806665	98.38%	10.559%
9	9.463	1251	1254	1265	rVB	306446	307878	7.96%	0.854%
10	9.745	1298	1302	1314	rVB	1462102	1416515	36.61%	3.929%
11	10.539	1432	1437	1451	rBV	3072418	3213307	83.05%	8.913%
12	11.227	1550	1554	1573	rVB	1360801	1276376	32.99%	3.540%
13	11.769	1642	1646	1668	rBV	603611	674424	17.43%	1.871%
14	12.545	1775	1778	1791	rBV	186451	246354	6.37%	0.683%
15	12.810	1818	1823	1827	rBV	3632755	3626078	93.72%	10.058%
16	13.051	1860	1864	1874	rBV3	25642	44531	1.15%	0.124%
17	13.727	1974	1979	1990	rBV2	249120	583198	15.07%	1.618%
18	13.857	1997	2001	2009	rVB	1100732	1021029	26.39%	2.832%
19	14.033	2027	2031	2035	rBV	76466	69814	1.80%	0.194%
20	14.339	2079	2083	2086	rBV	113068	111511	2.88%	0.309%
21	14.633	2129	2133	2138	rBV	140361	143292	3.70%	0.397%
22	14.945	2182	2186	2191	rBV	155014	175848	4.54%	0.488%
23	15.268	2236	2241	2244	rBV	738890	885357	22.88%	2.456%
24	15.298	2244	2246	2252	rVB	136441	155384	4.02%	0.431%
25	15.704	2310	2315	2320	rVB	109477	152147	3.93%	0.422%
26	15.798	2326	2331	2332	rBV4	33352	49606	1.28%	0.138%
27	16.168	2389	2394	2398	rBV2	55164	99335	2.57%	0.276%

Sum of corrected areas: 36052582

LSC Report - Integrated Chromatogram

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Data File : BF113237.D
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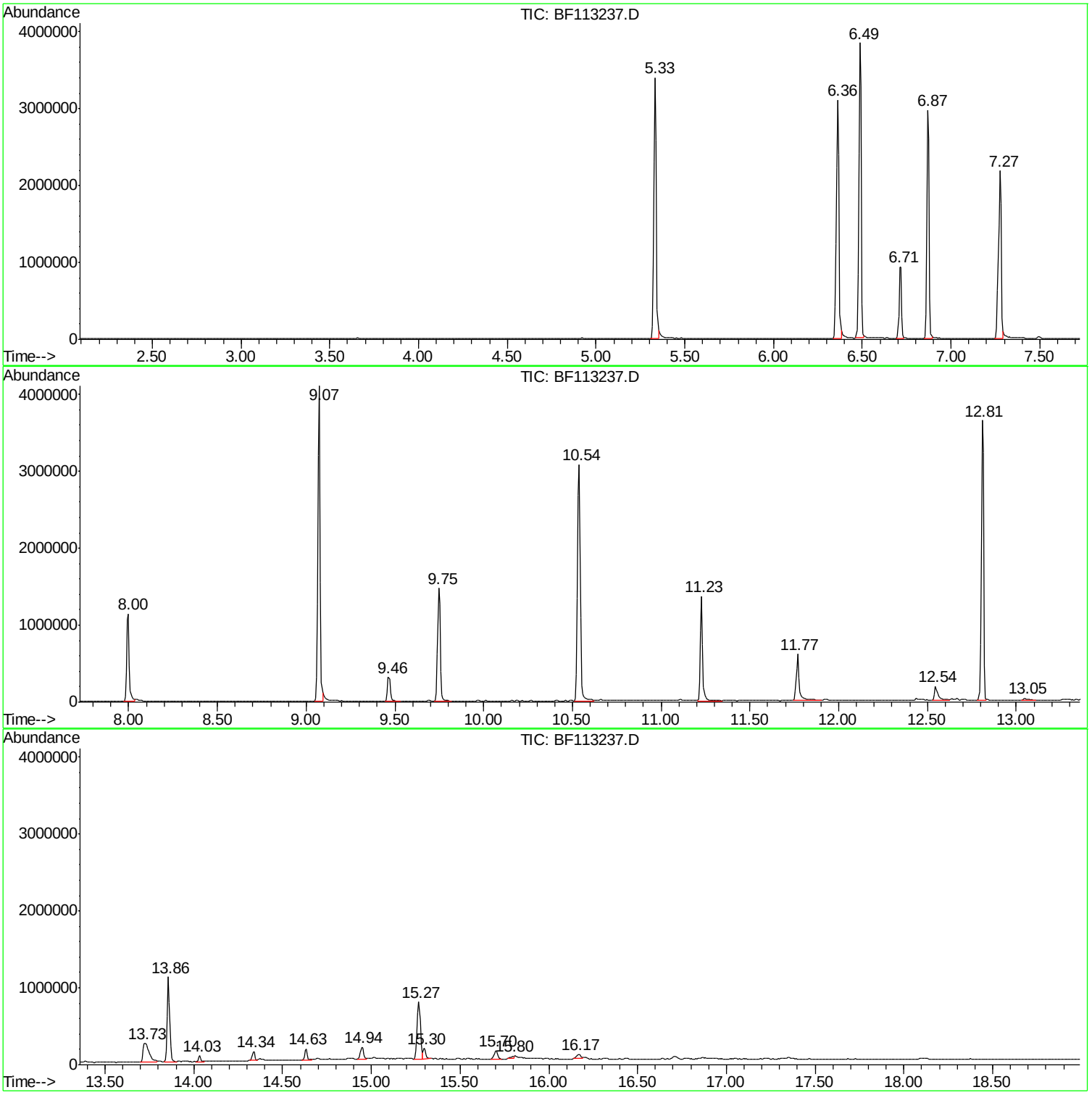
Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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

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Data File : BF113237.D
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

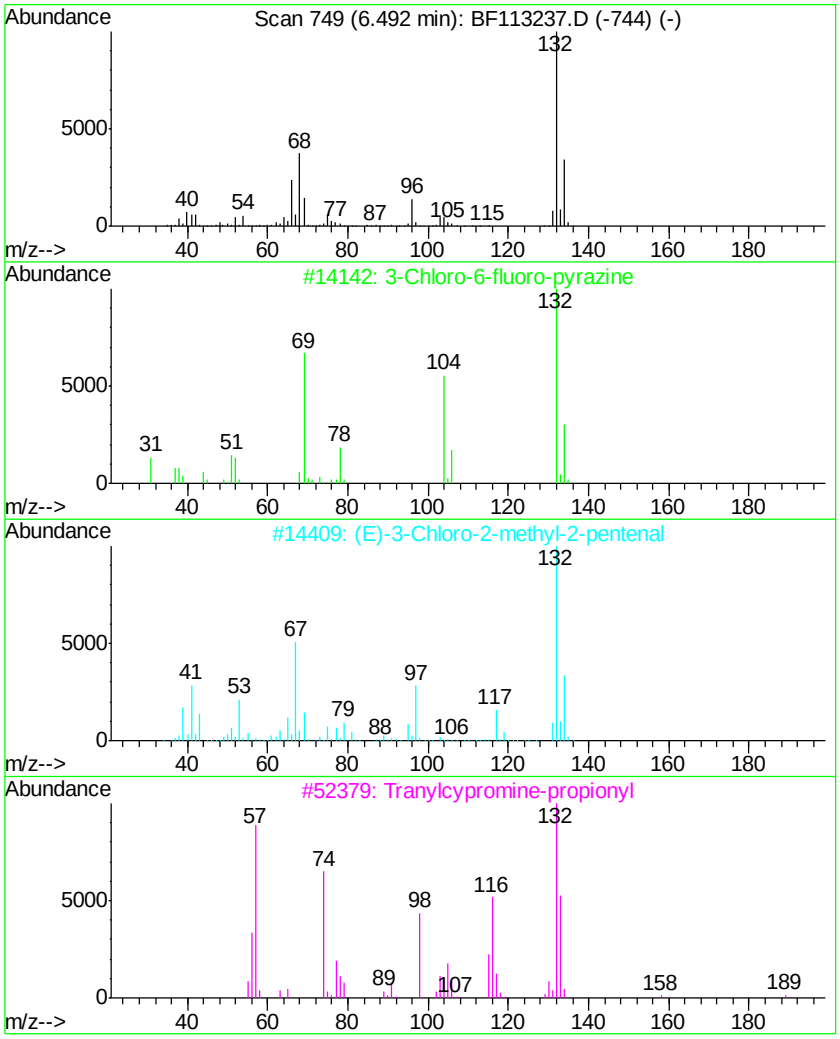
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

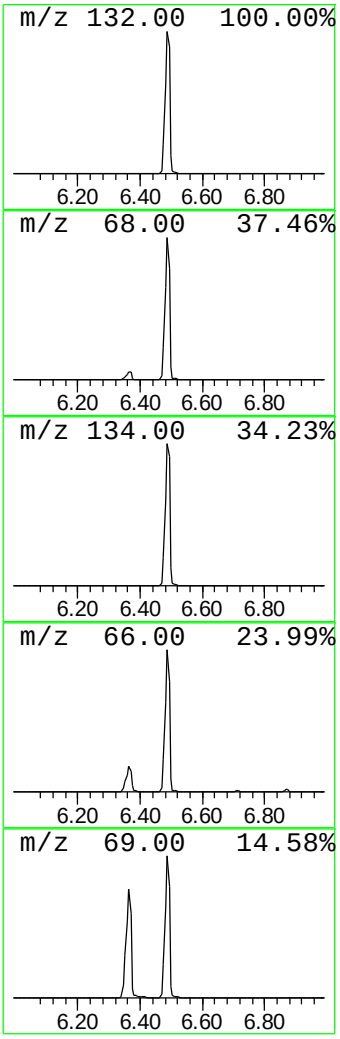
****

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	88.66 ng	3869160	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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BF113237.D
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Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

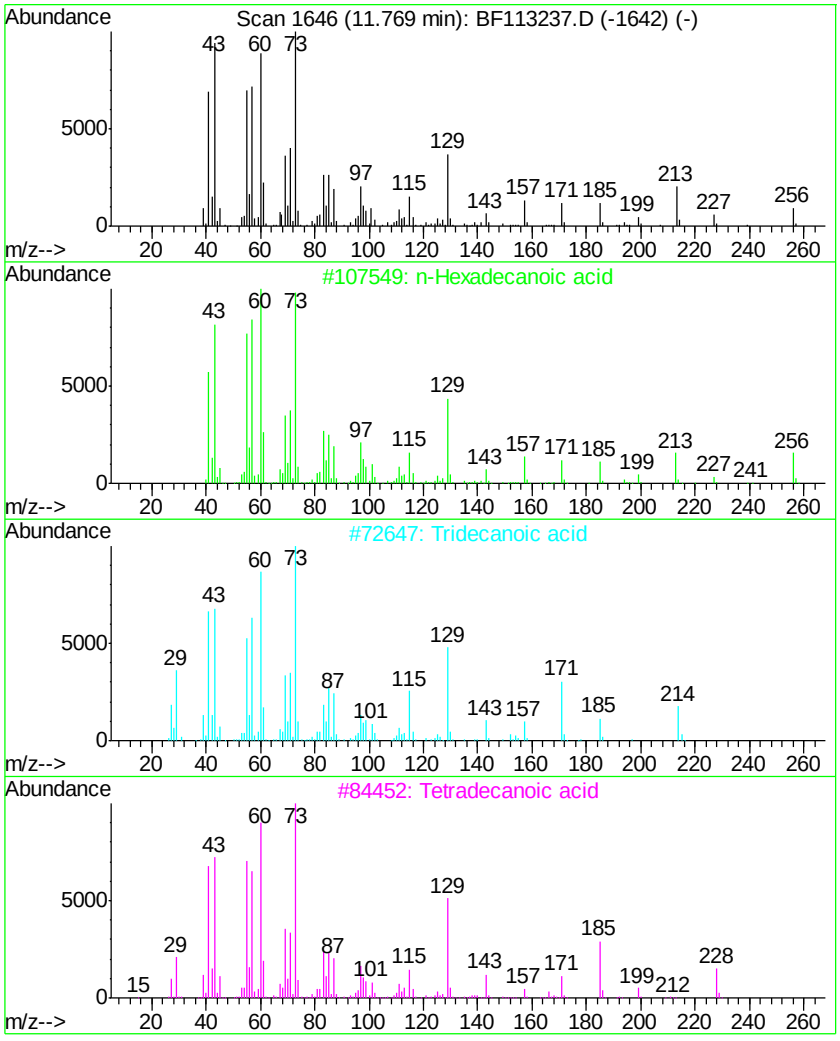
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

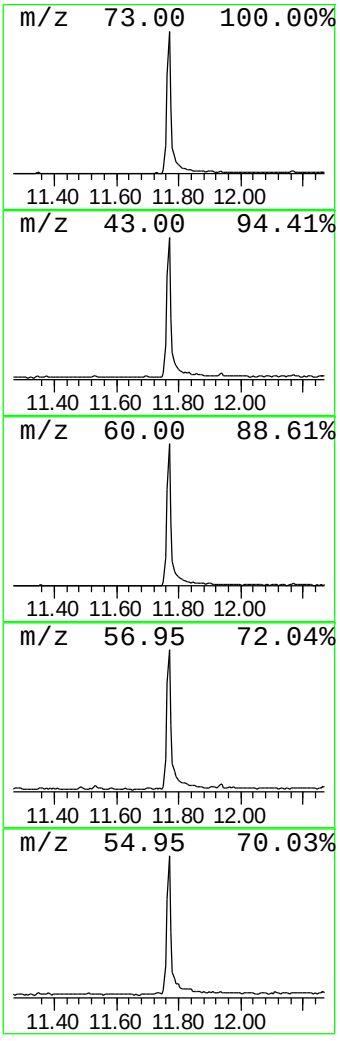
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	10.57 ng	674424	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113237.D
Acq On : 22 Mar 2019 16:25
Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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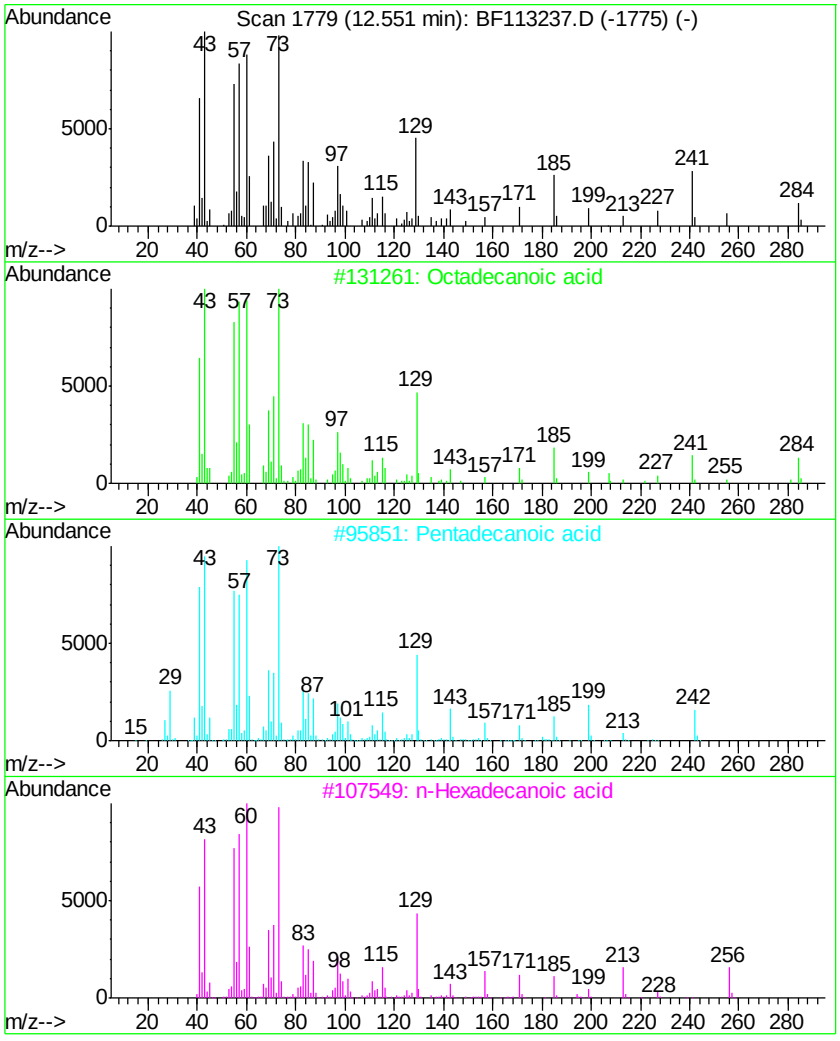
TIC Integration Parameters: LSCINT.P

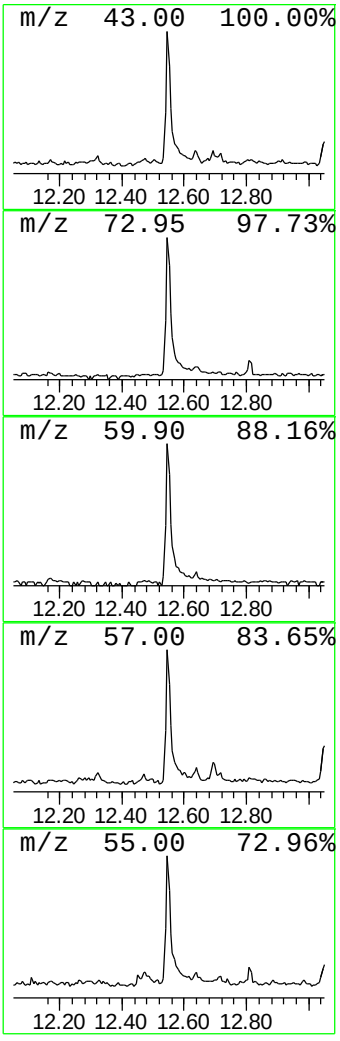
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	4.83 ng	246354	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113237.D
Acq On : 22 Mar 2019 16:25
Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

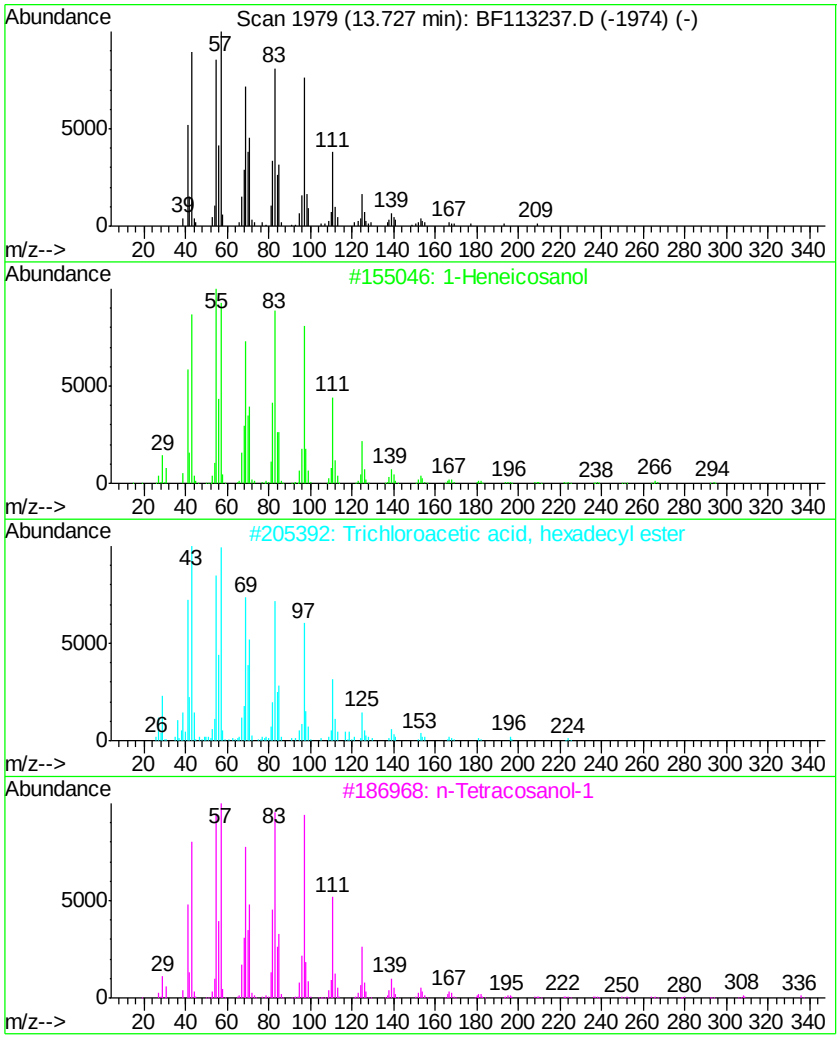
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

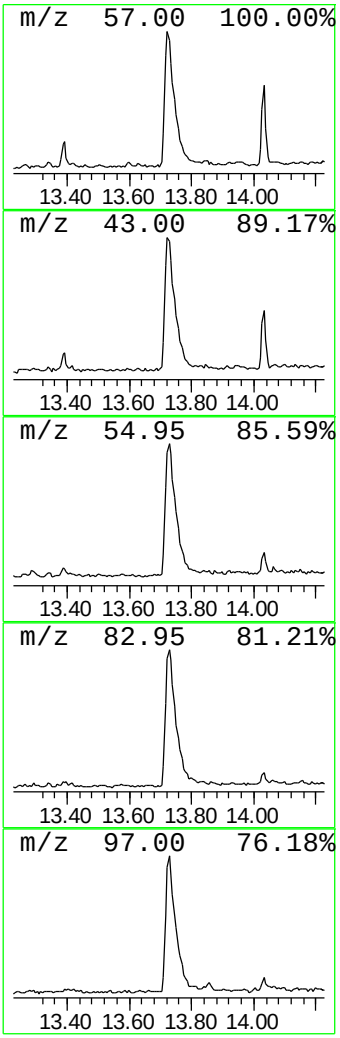
****

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	11.42 ng	583198	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113237.D
Acq On : 22 Mar 2019 16:25
Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

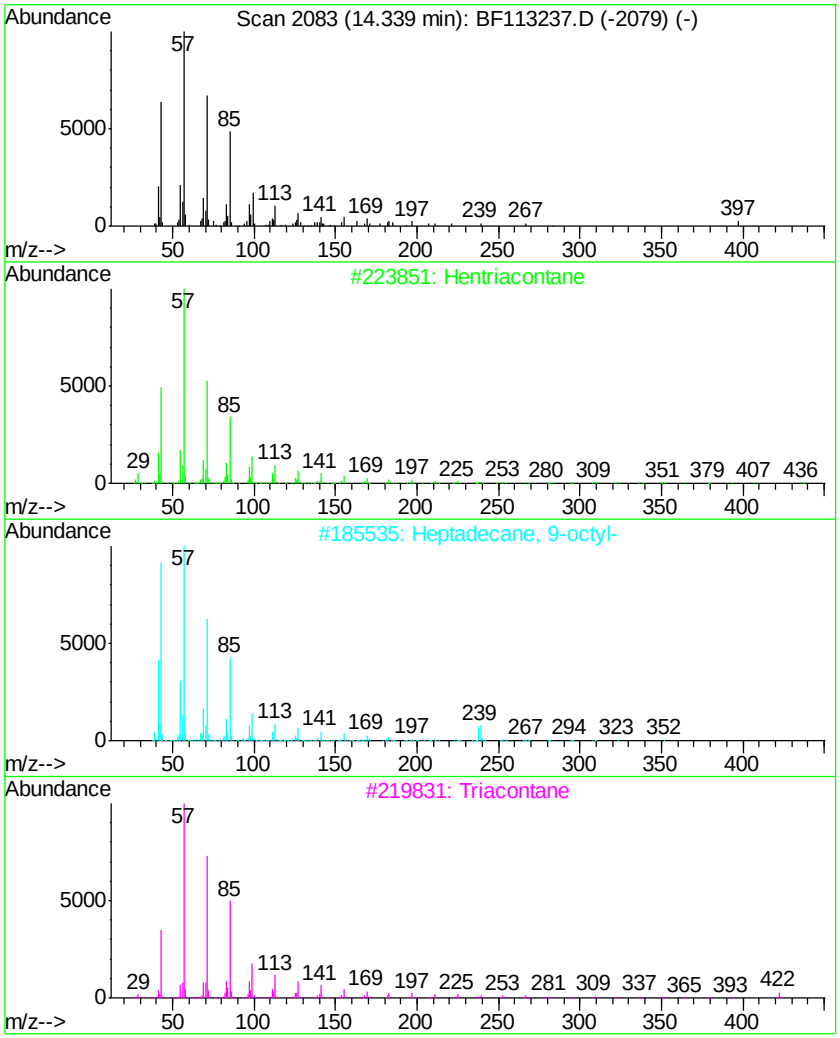
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

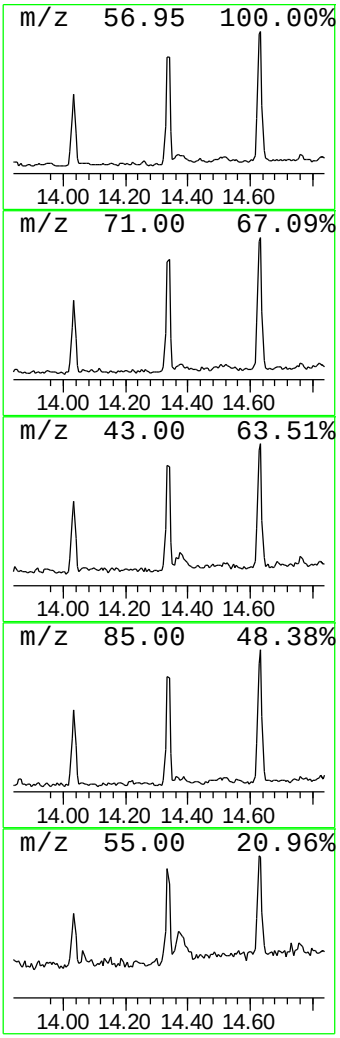
****

Peak Number 6 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.18 ng	111511	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Data File : BF113237.D
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Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

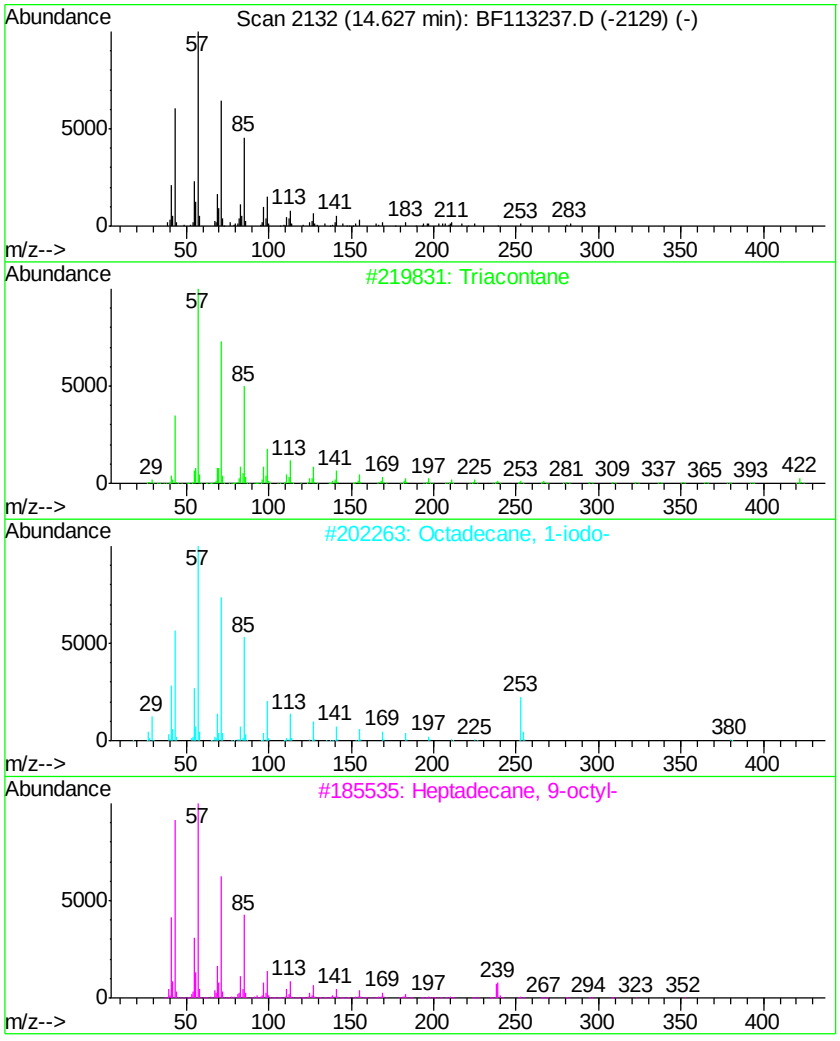
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

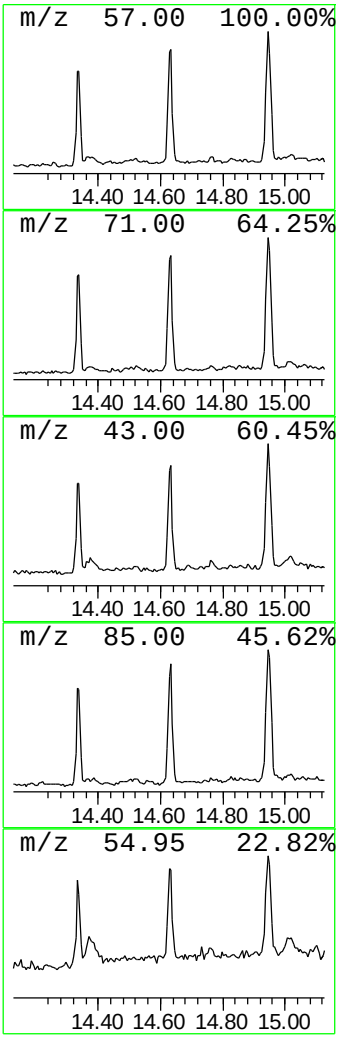
****

Peak Number 7 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	3.24 ng	143292	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Docosane	310	C22H46	000629-97-0	91
5	Hexacosane	366	C26H54	000630-01-3	90





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Sample : K2018-05
Misc :
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Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

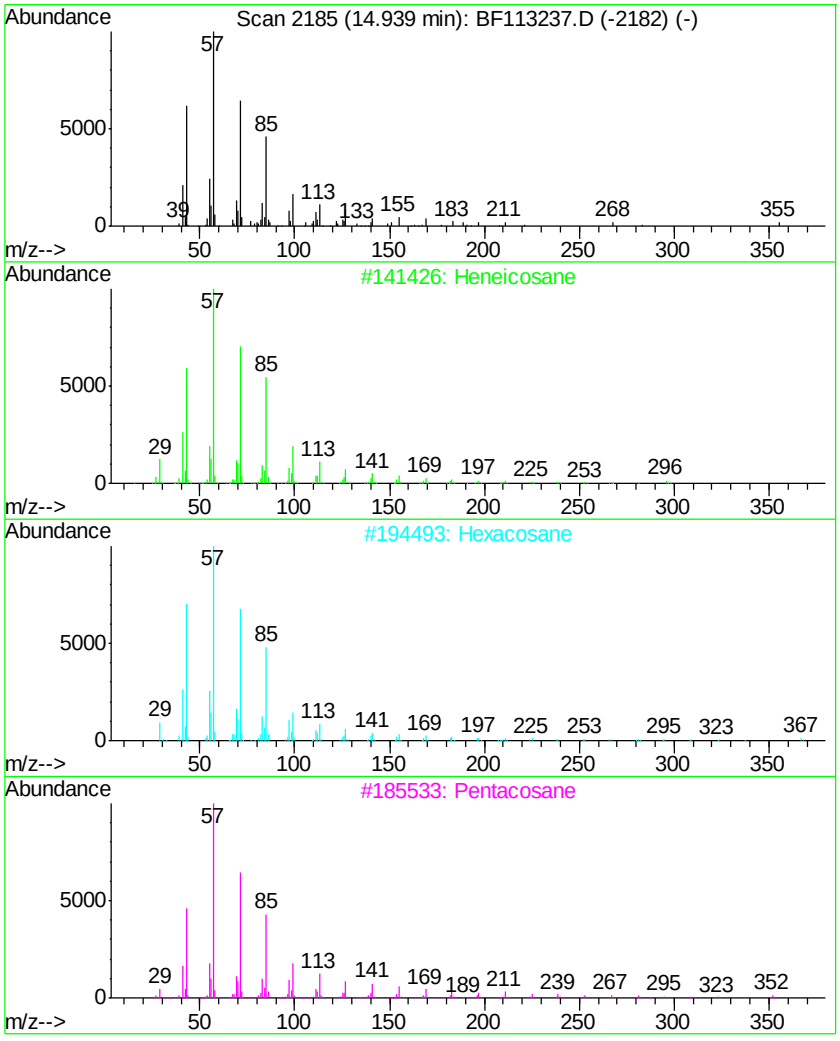
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

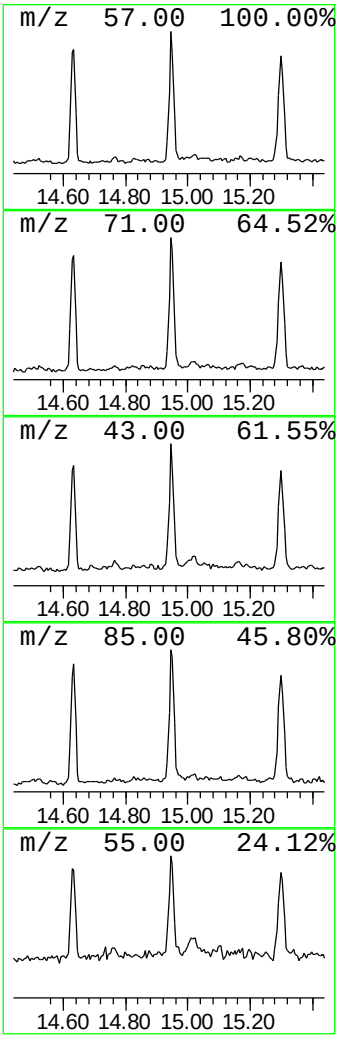
****

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	3.97 ng	175848	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Pentacosane	352	C25H52	000629-99-2	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87





Library Search Compound Report

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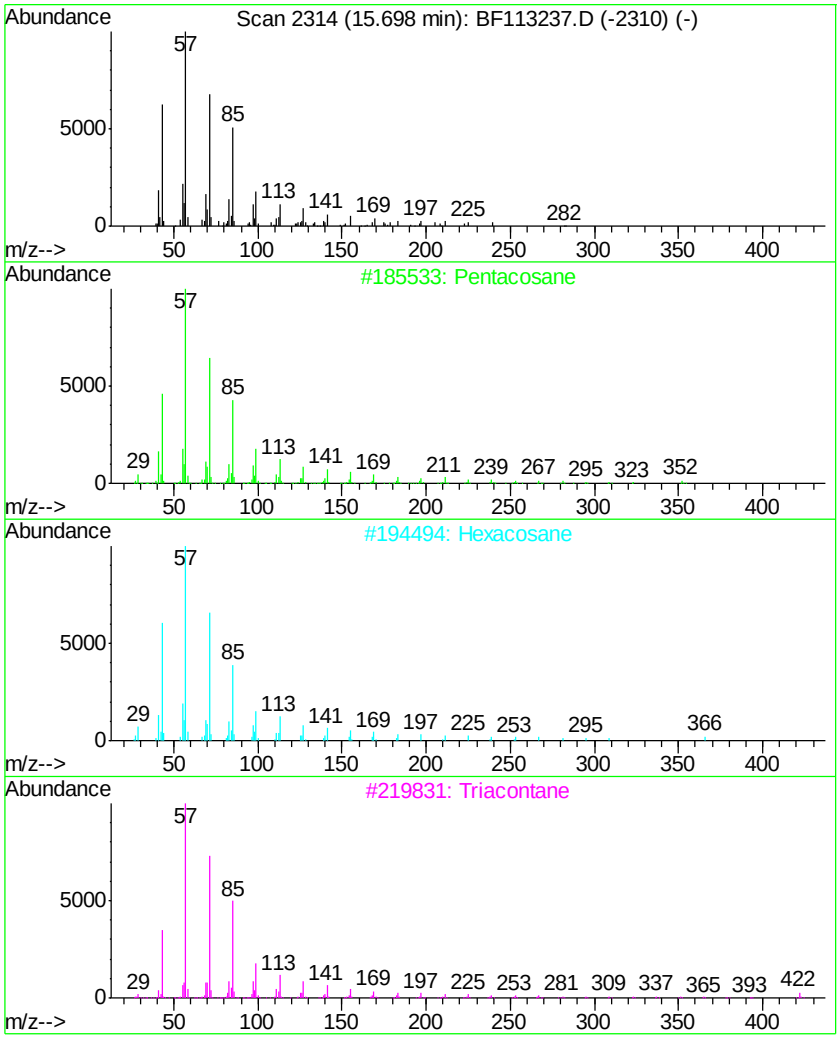
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

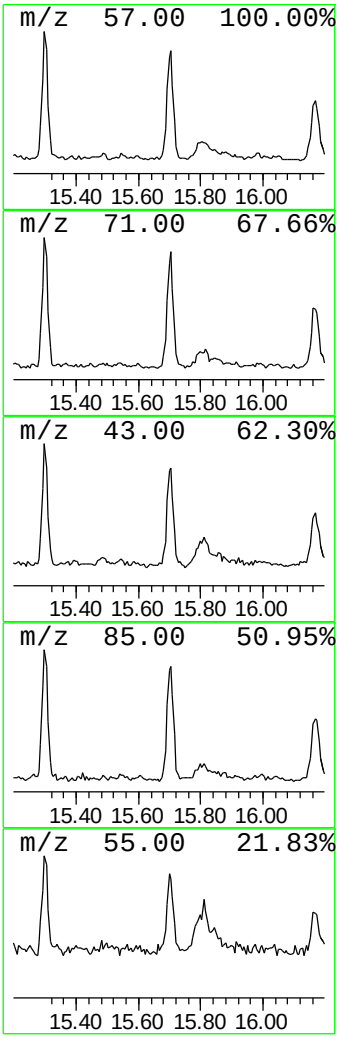
****

Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	3.44 ng	152147	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





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Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

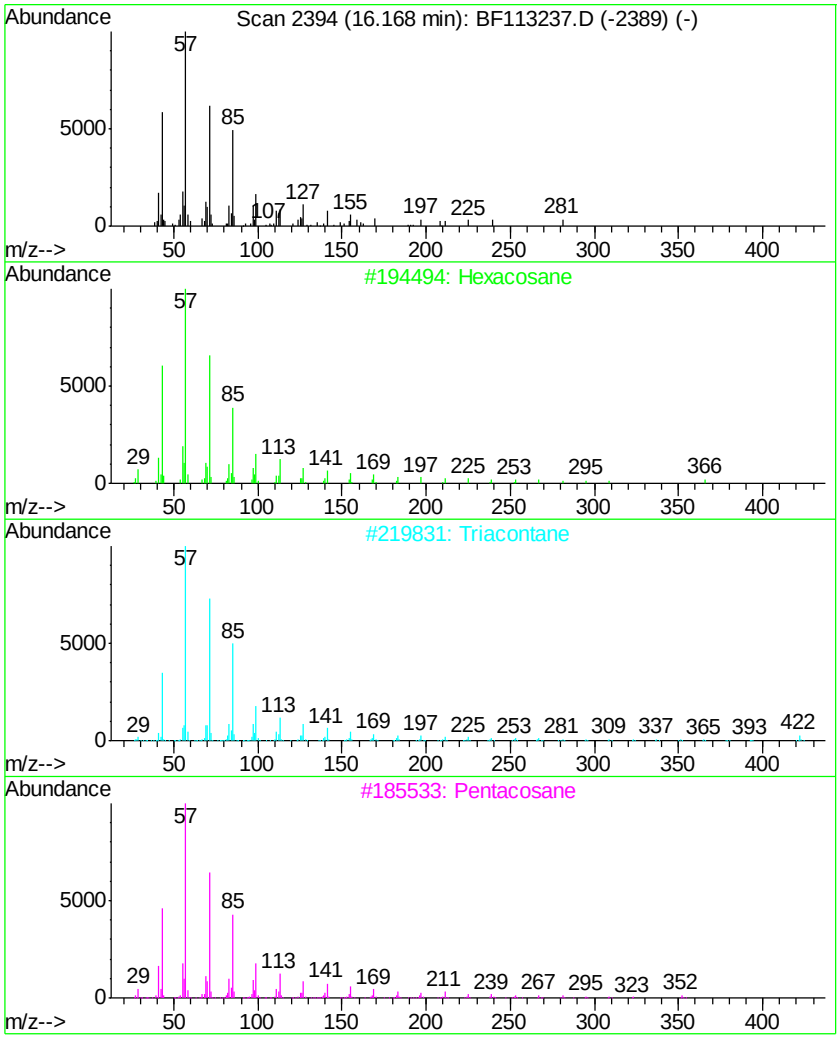
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

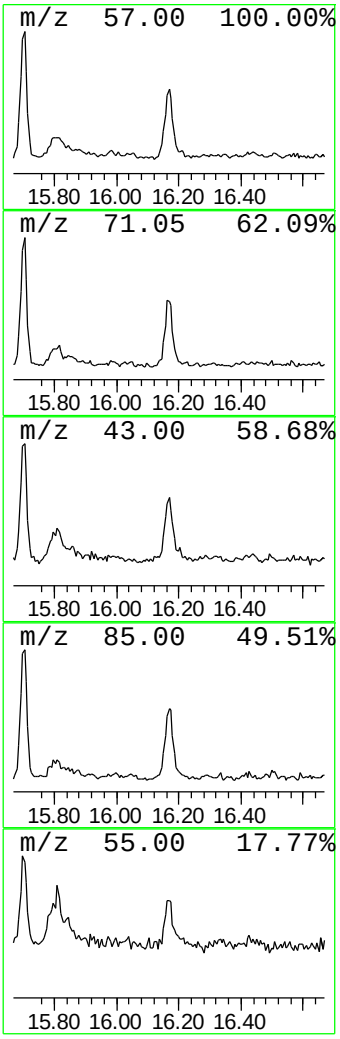
****

Peak Number 10 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.24 ng	99335	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Triacontane	422	C30H62	000638-68-6	87
3	Pentacosane	352	C25H52	000629-99-2	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptacosane	380	C27H56	000593-49-7	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113237.D
Acq On : 22 Mar 2019 16:25
Operator : JU/SJ
Sample : K2018-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.49	6.49	88.7	ng	3869160	1	6.72	872818	20.0
n-Hexadecanoic acid	11.77	10.6	ng	674424	4	11.23	1276380	20.0
Octadecanoic acid	12.55	4.8	ng	246354	5	13.86	1021030	20.0
1-Heneicosanol	13.73	11.4	ng	583198	5	13.86	1021030	20.0
Hentriacontane	14.34	2.2	ng	111511	5	13.86	1021030	20.0
Triacontane	14.63	3.2	ng	143292	6	15.27	885357	20.0
Heneicosane	14.94	4.0	ng	175848	6	15.27	885357	20.0
Pentacosane	15.70	3.4	ng	152147	6	15.27	885357	20.0
Hexacosane	16.17	2.2	ng	99335	6	15.27	885357	20.0