LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113236.D
Acq On : 22 Mar 2019 15:56
Operator : JU/SJ
Sample : K2018-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-B

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	3158762	3077209	87.78%	9.329%
2	6.363	722	727	744	rBV	3106605	3505758	100.00%	10.628%
3	6.487	744	748	751	rBV	3638441	3311020	94.45%	10.038%
4	6.716	783	787	797	rBV	933335	856004	24.42%	2.595%
5	6.869	809	813	817	rBV	2698806	2460153	70.17%	7.458%
6	7.275	877	882	885	rBV	2130426	2133686	60.86%	6.468%
7	7.998	1000	1005	1012	rBV	1166502	1151050	32.83%	3.489%
8	8.616	1108	1110	1120	rVB	37421	37155	1.06%	0.113%
9	9.075	1183	1188	1191	rBV	3830438	3389667	96.69%	10.276%
10	9.469	1250	1255	1265	rBV	260564	261798	7.47%	0.794%
11	9.745	1298	1302	1311	rBV	1405307	1338639	38.18%	4.058%
12	10.533	1432	1436	1451	rBV	2440264	2671939	76.22%	8.100%
13	11.227	1550	1554	1564	rBV	1506264	1377737	39.30%	4.177%
14	11.769	1642	1646	1657	rBV	428497	520127	14.84%	1.577%
15	12.545	1775	1778	1789	rBV	135488	176495	5.03%	0.535%
16	12.810	1818	1823	1826	rBV	3511138	3499315	99.82%	10.608%
17	13.727	1974	1979	1995	rBV2	144521	361918	10.32%	1.097%
18	13.857	1997	2001	2009	rVB	1258756	1163282	33.18%	3.527%
19	14.033	2028	2031	2033	rBV	44078	38192	1.09%	0.116%
20	14.333	2079	2082	2086	rBV	70048	63679	1.82%	0.193%
21	14.633	2129	2133	2136	rBV	99477	99022	2.82%	0.300%
22	14.945	2182	2186	2192	rBV	122398	134918	3.85%	0.409%
23	15.268	2236	2241	2244	rBV	722705	875702	24.98%	2.655%
24	15.298	2244	2246	2252	rVB	114589	132842	3.79%	0.403%
25	15.704	2310	2315	2319	rVB	110646	151131	4.31%	0.458%
26	15.804	2327	2332	2337	rBV9	21043	49908	1.42%	0.151%
27	16.168	2389	2394	2400	rBV3	51125	88354	2.52%	0.268%
28	16.709	2482	2486	2492	rVB3	31456	59512	1.70%	0.180%

Sum of corrected areas: 32986212

LSC Report - Integrated Chromatogram

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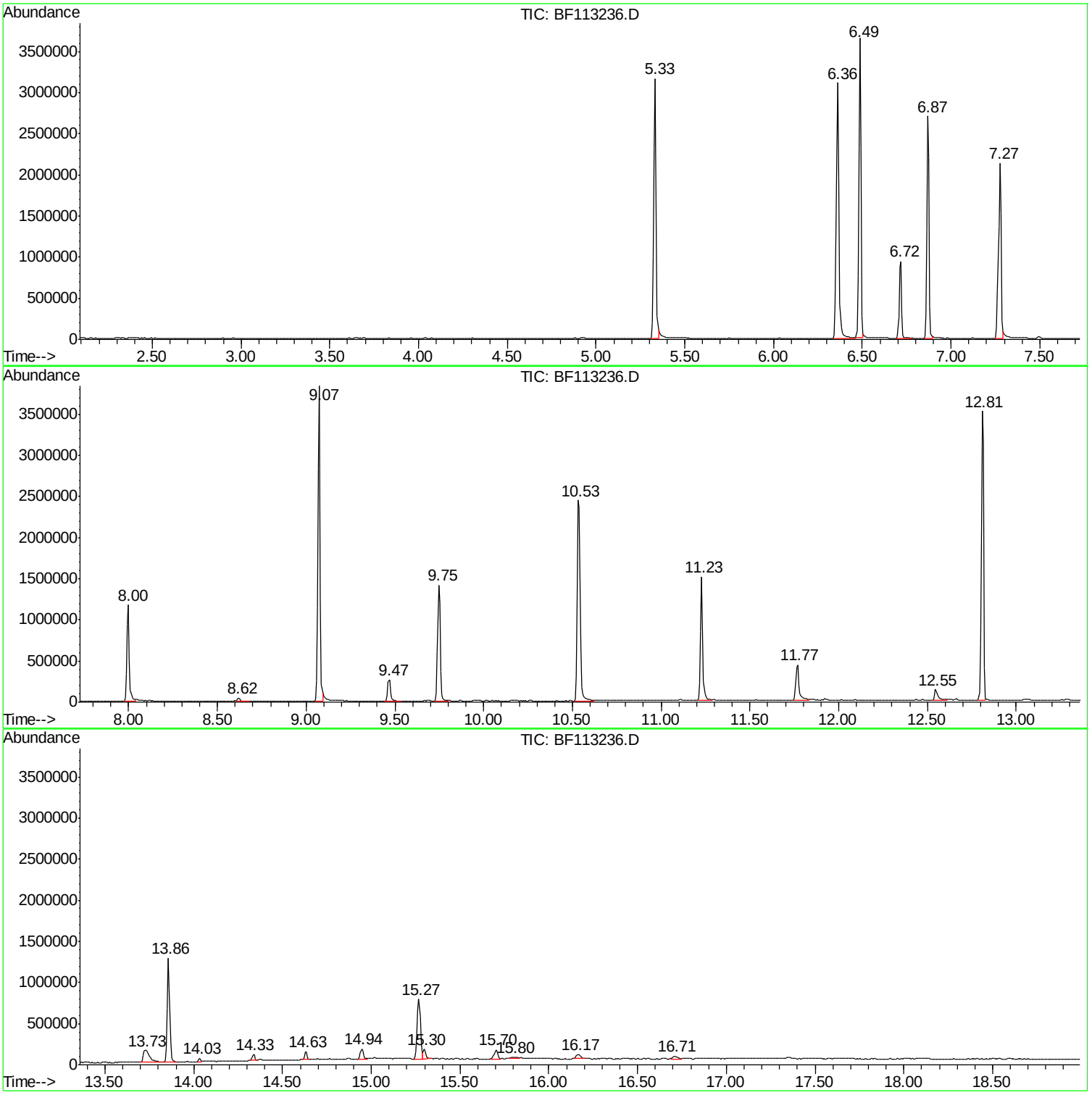
Operator : JU/SJ
Sample : K2018-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-B

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032219\
Data File : BF113236.D
Acq On : 22 Mar 2019 15:56
Operator : JU/SJ
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ClientSampleId : SP-1-B

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

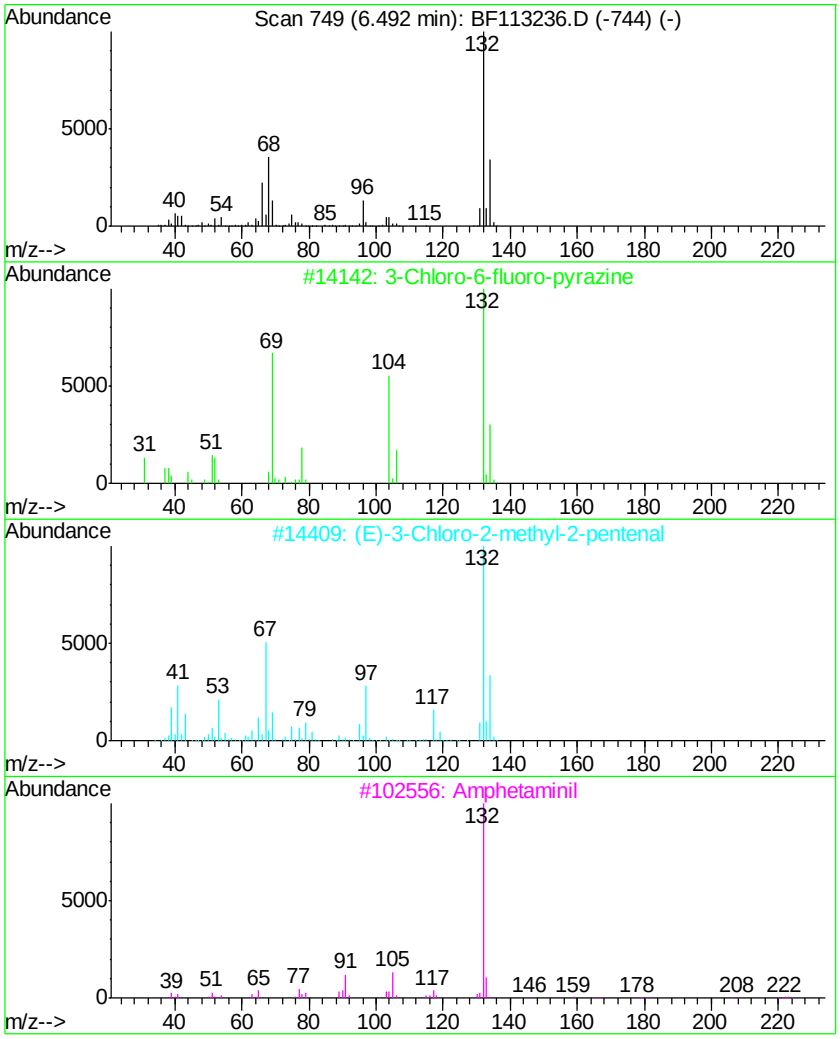
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

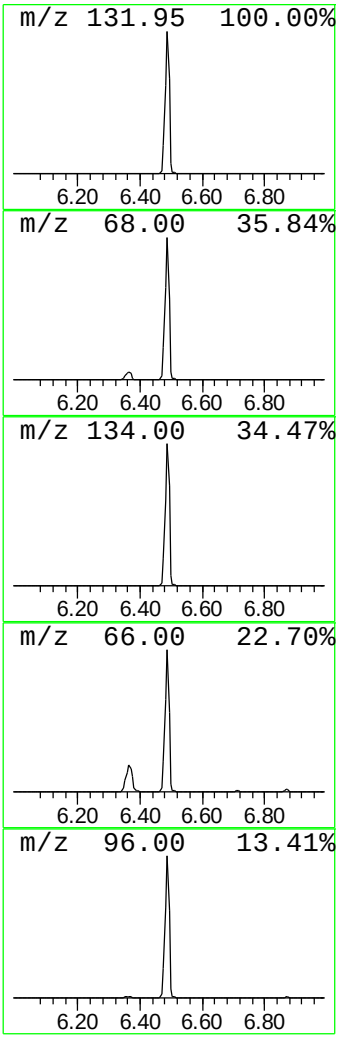
****

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	77.36 ng	3311020	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	Amphetaminil	250	C17H18N2	017590-01-1	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

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Data File : BF113236.D
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Operator : JU/SJ
Sample : K2018-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-B

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

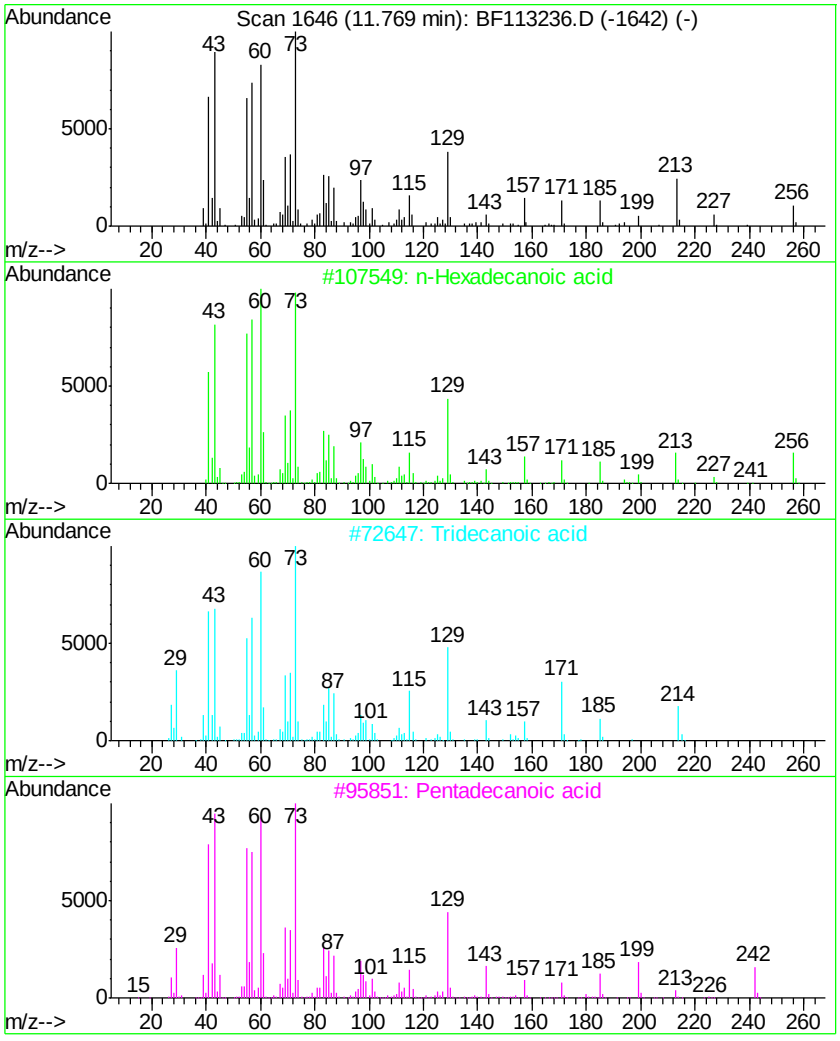
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

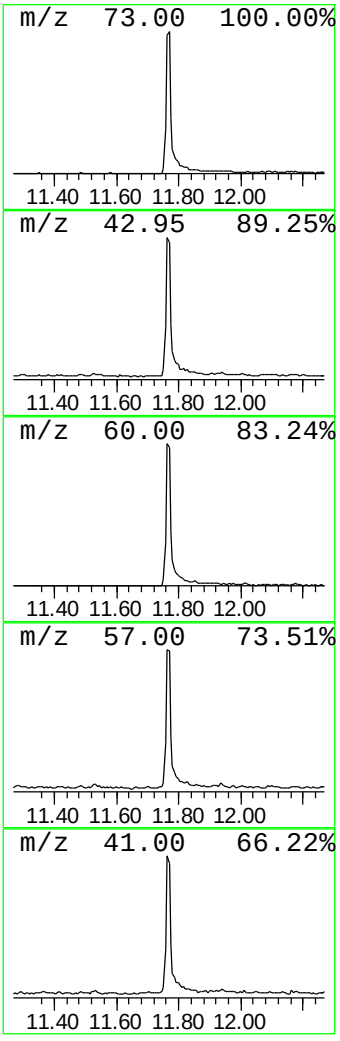
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	7.55 ng	520127	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	97
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Sample : K2018-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-B

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

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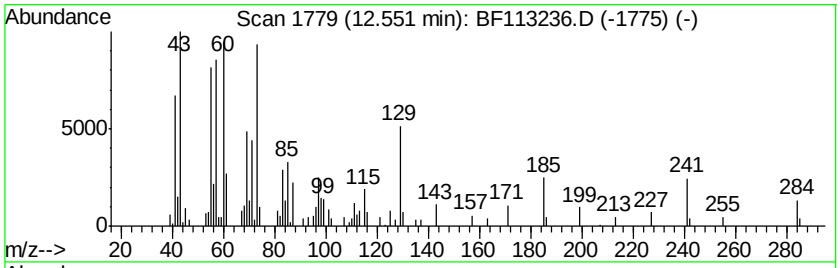
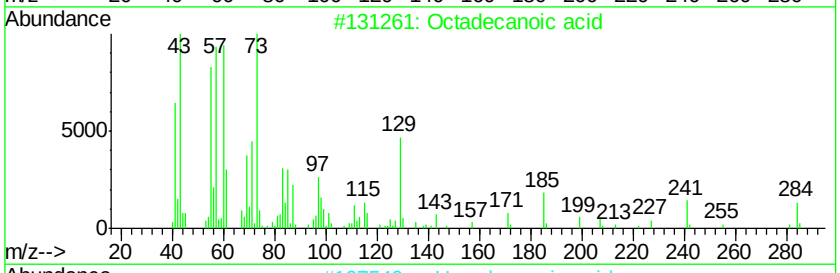
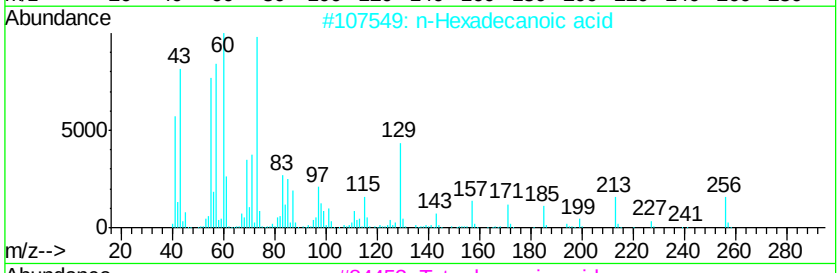
Peak Number 4 Octadecanoic acid Concentration Rank 7

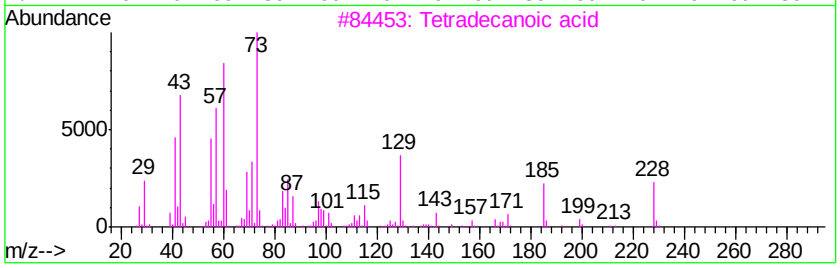
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	3.03 ng	176495	Chrysene-d12	13.86

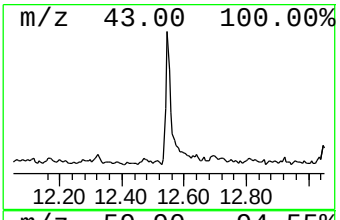
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49

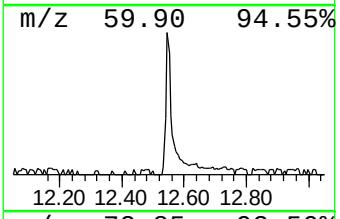


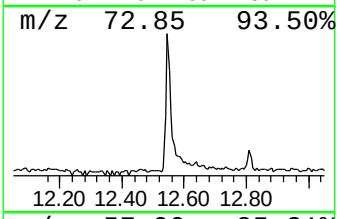


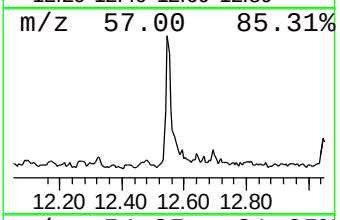


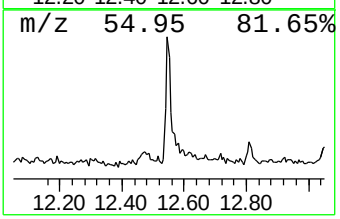












Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-1-B

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

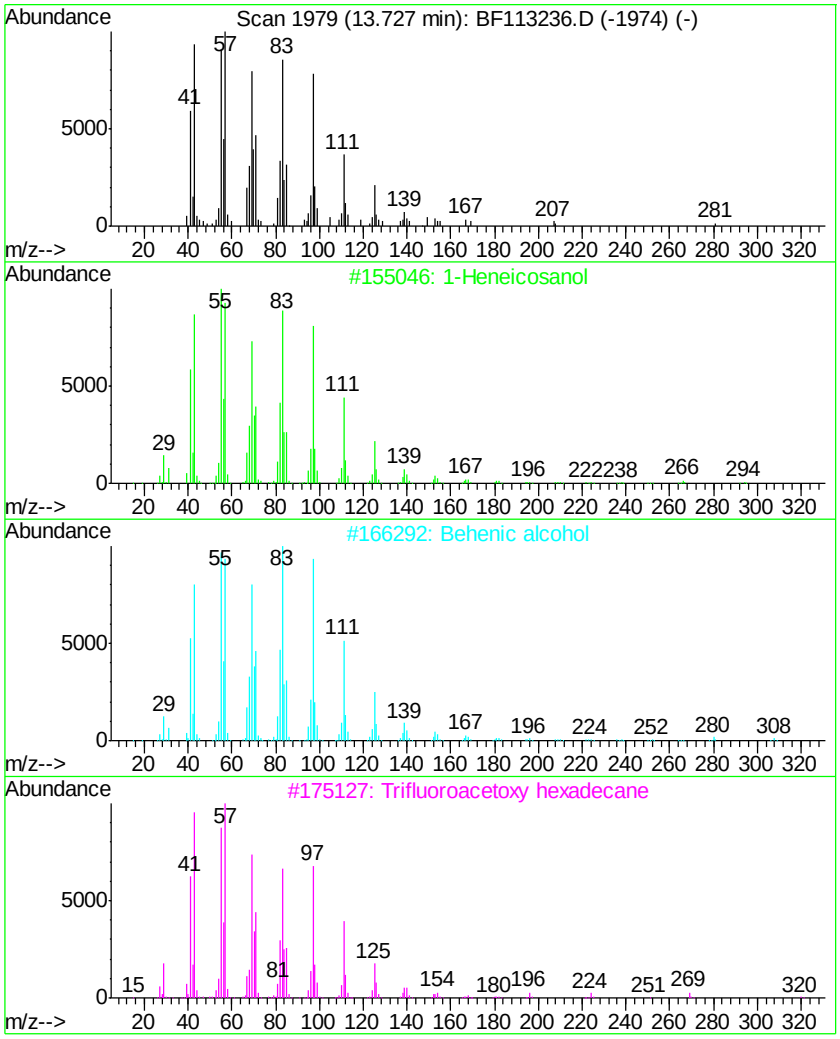
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

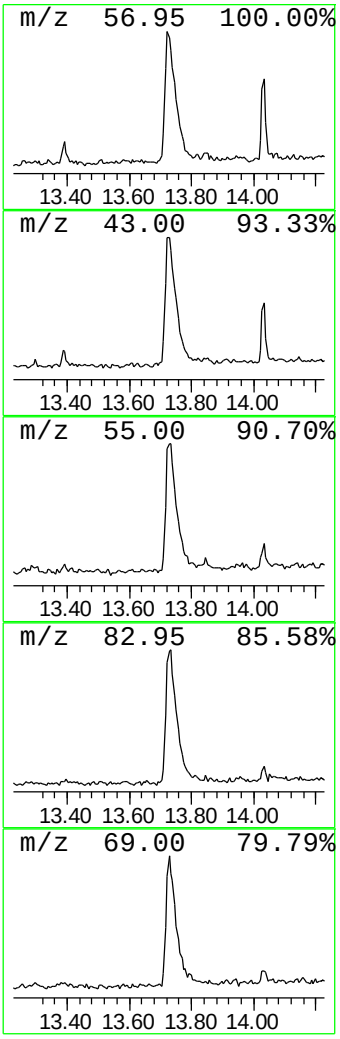
****

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.22 ng	361918	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91





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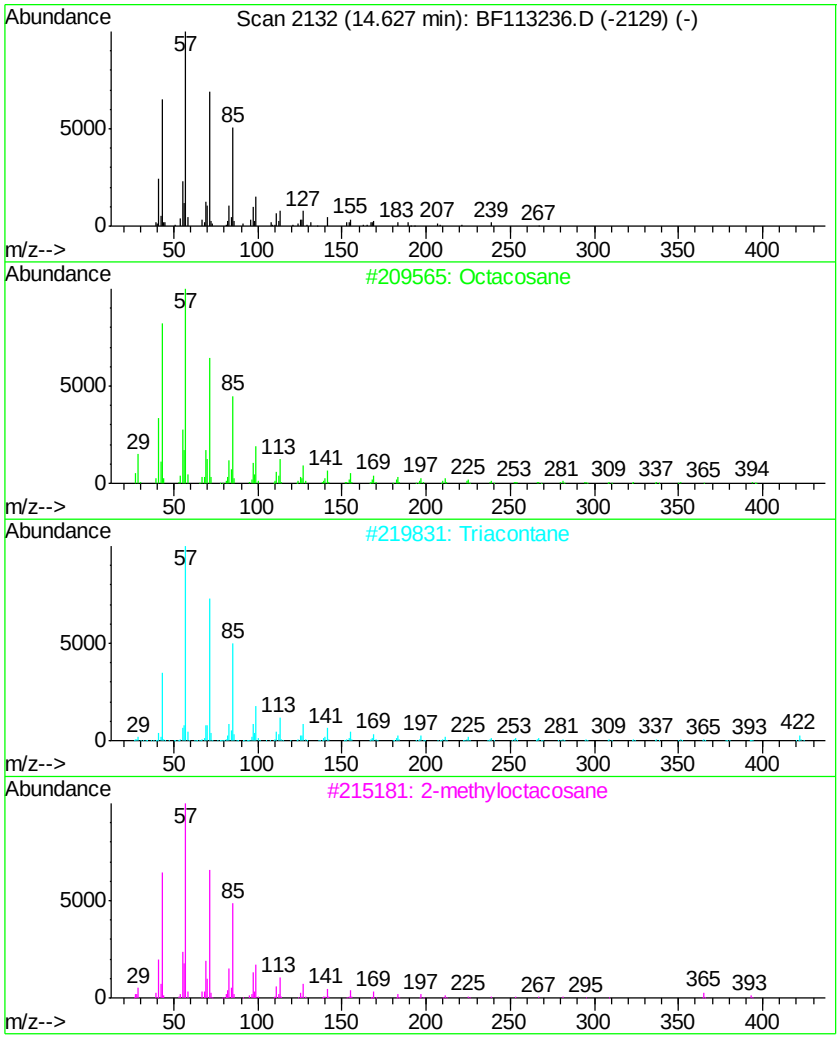
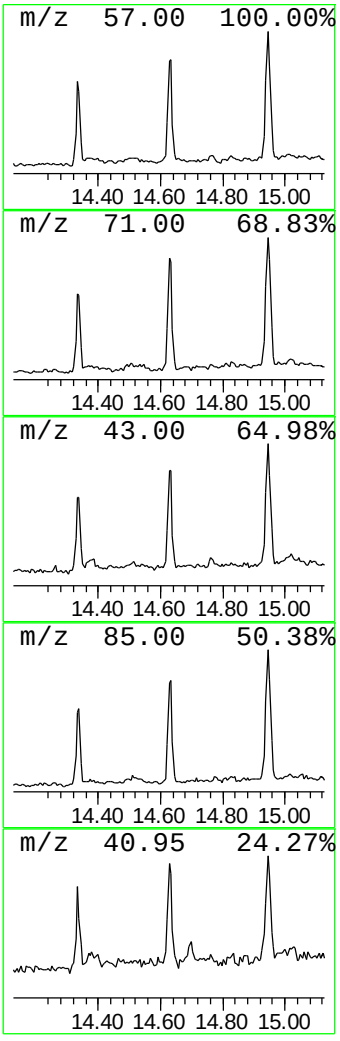
****

Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.26 ng	99022	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Triacontane	422	C30H62	000638-68-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane	296	C21H44	000629-94-7	90





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TIC Library : C:\DATABASE\NIST11.L
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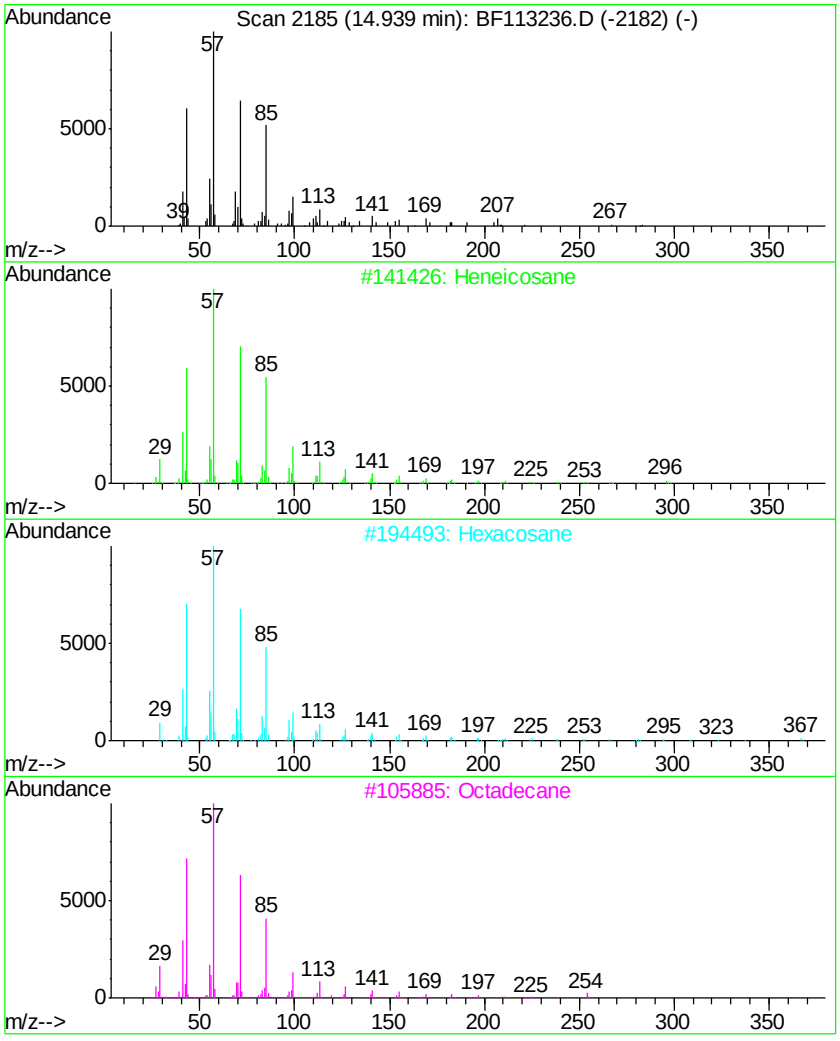
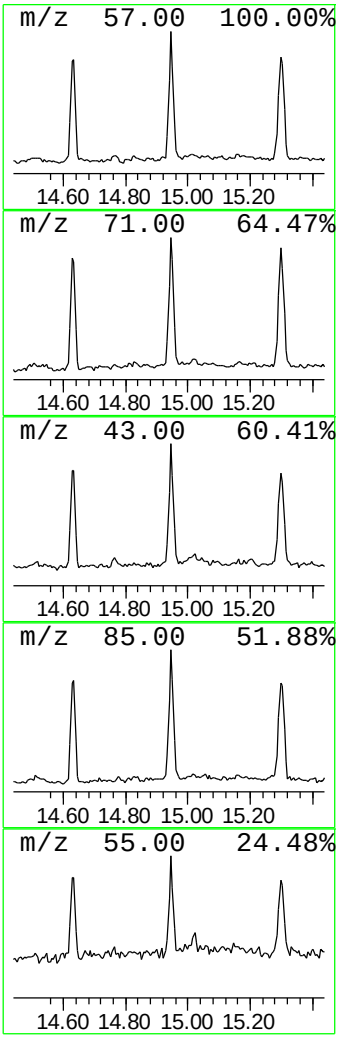
Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	3.08 ng	134918	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octadecane	254	C18H38	000593-45-3	87
4	Nonadecane	268	C19H40	000629-92-5	87
5	Tetracosane	338	C24H50	000646-31-1	81





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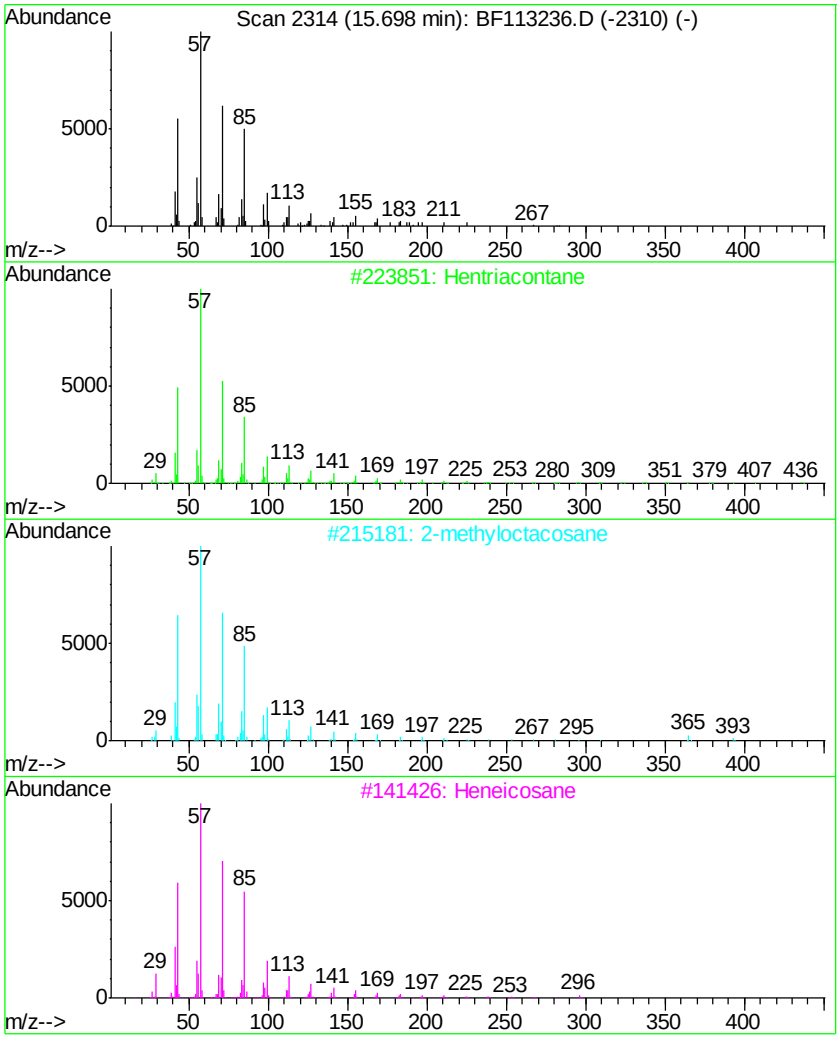
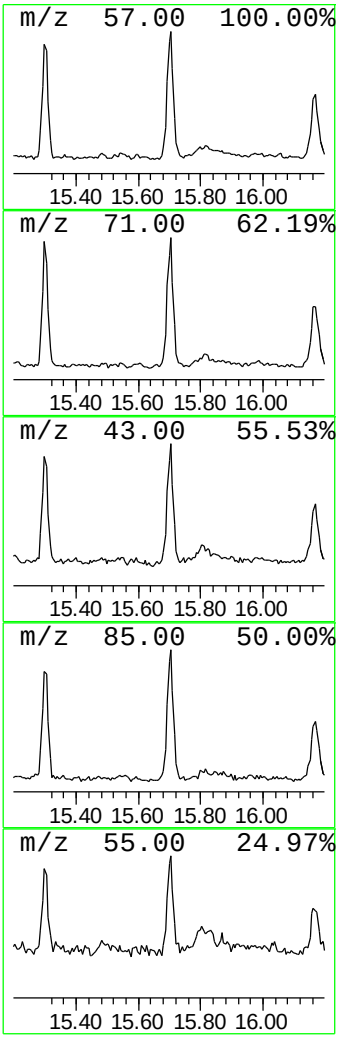
Peak Number 8 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	3.45 ng	151131	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane	240	C17H36	000629-78-7	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

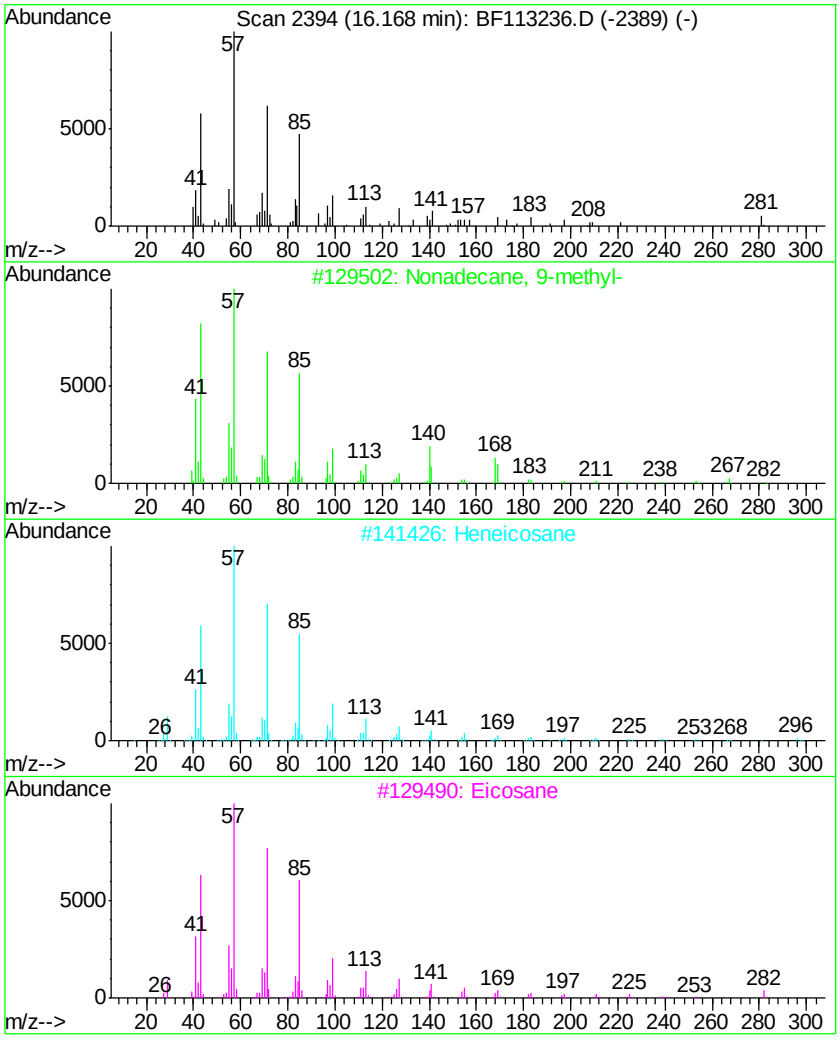
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

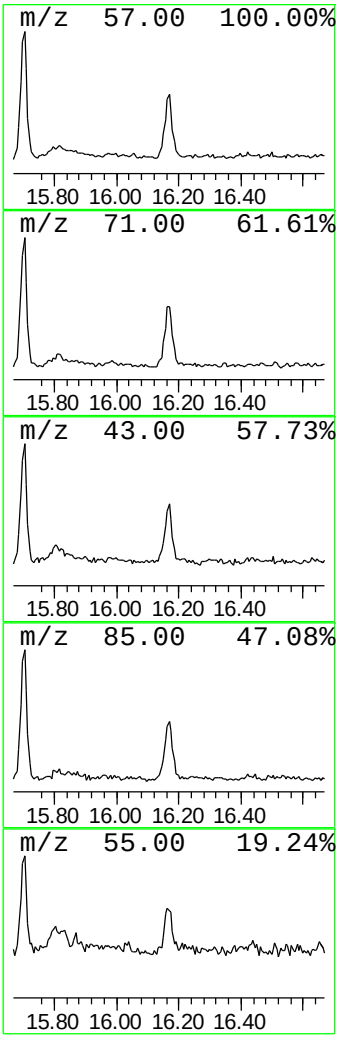
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.02 ng	88354	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.49	6.49	77.4	ng	3311020	1	6.72	856004	20.0
n-Hexadecanoic acid	11.77	7.5	ng	520127	4	11.23	1377740	20.0
Octadecanoic acid	12.55	3.0	ng	176495	5	13.86	1163280	20.0
1-Heneicosanol	13.73	6.2	ng	361918	5	13.86	1163280	20.0
Octacosane	14.63	2.3	ng	99022	6	15.27	875702	20.0
Heneicosane	14.94	3.1	ng	134918	6	15.27	875702	20.0
Hentriacontane	15.70	3.5	ng	151131	6	15.27	875702	20.0
Nonadecane, 9-met...	16.17	2.0	ng	88354	6	15.27	875702	20.0