LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113086.D
Acq On : 18 Mar 2019 13:21
Operator : JU/SJ
Sample : K1933-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-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:\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	5.345	549	554	557	rBV	3383424	3344664	14.76%	5.058%
2	6.375	724	729	732	rBV	3561571	3962086	17.48%	5.991%
3	6.504	746	751	754	rBV	4085213	4008080	17.68%	6.061%
4	6.728	785	789	792	rBV	1375391	1129284	4.98%	1.708%
5	6.886	808	816	819	rBV	3404153	3059002	13.50%	4.626%
6	7.286	879	884	887	rBV	2499511	2491873	10.99%	3.768%
7	8.010	1003	1007	1013	rBV	1466763	1367078	6.03%	2.067%
8	9.086	1185	1190	1204	rBV	4170885	4227851	18.65%	6.393%
9	9.475	1252	1256	1267	rBV	488604	463048	2.04%	0.700%
10	9.757	1300	1304	1318	rBV2	1852568	1729868	7.63%	2.616%
11	10.545	1433	1438	1453	rBV	3269652	3327580	14.68%	5.032%
12	11.239	1552	1556	1558	rBV	1765230	1743462	7.69%	2.636%
13	11.780	1643	1648	1651	rBV	1195651	1294230	5.71%	1.957%
14	12.445	1758	1761	1764	rBV	388926	334600	1.48%	0.506%
15	12.557	1776	1780	1788	rBV	689196	761664	3.36%	1.152%
16	12.668	1796	1799	1803	rVB	255046	244526	1.08%	0.370%
17	12.821	1820	1825	1828	rBV	3900448	3781239	16.68%	5.718%
18	13.704	1972	1975	1978	rBV	474554	466743	2.06%	0.706%
19	13.751	1980	1983	1993	rVB3	279253	615579	2.72%	0.931%
20	13.886	1997	2006	2009	rBV2	9613735	22666677	100.00%	34.276%
21	14.345	2081	2084	2088	rBV2	342739	343167	1.51%	0.519%
22	14.639	2131	2134	2138	rVB	473377	450117	1.99%	0.681%
23	14.957	2184	2188	2194	rVV	566957	650406	2.87%	0.984%
24	15.274	2237	2242	2245	rBV	1138344	1367567	6.03%	2.068%
25	15.309	2245	2248	2256	rVB	620992	811376	3.58%	1.227%
26	15.709	2312	2316	2322	rVB	470208	715646	3.16%	1.082%
27	16.180	2391	2396	2407	rVB2	280941	529154	2.33%	0.800%
28	16.727	2485	2489	2495	rVB	133137	243364	1.07%	0.368%

Sum of corrected areas: 66129931

LSC Report - Integrated Chromatogram

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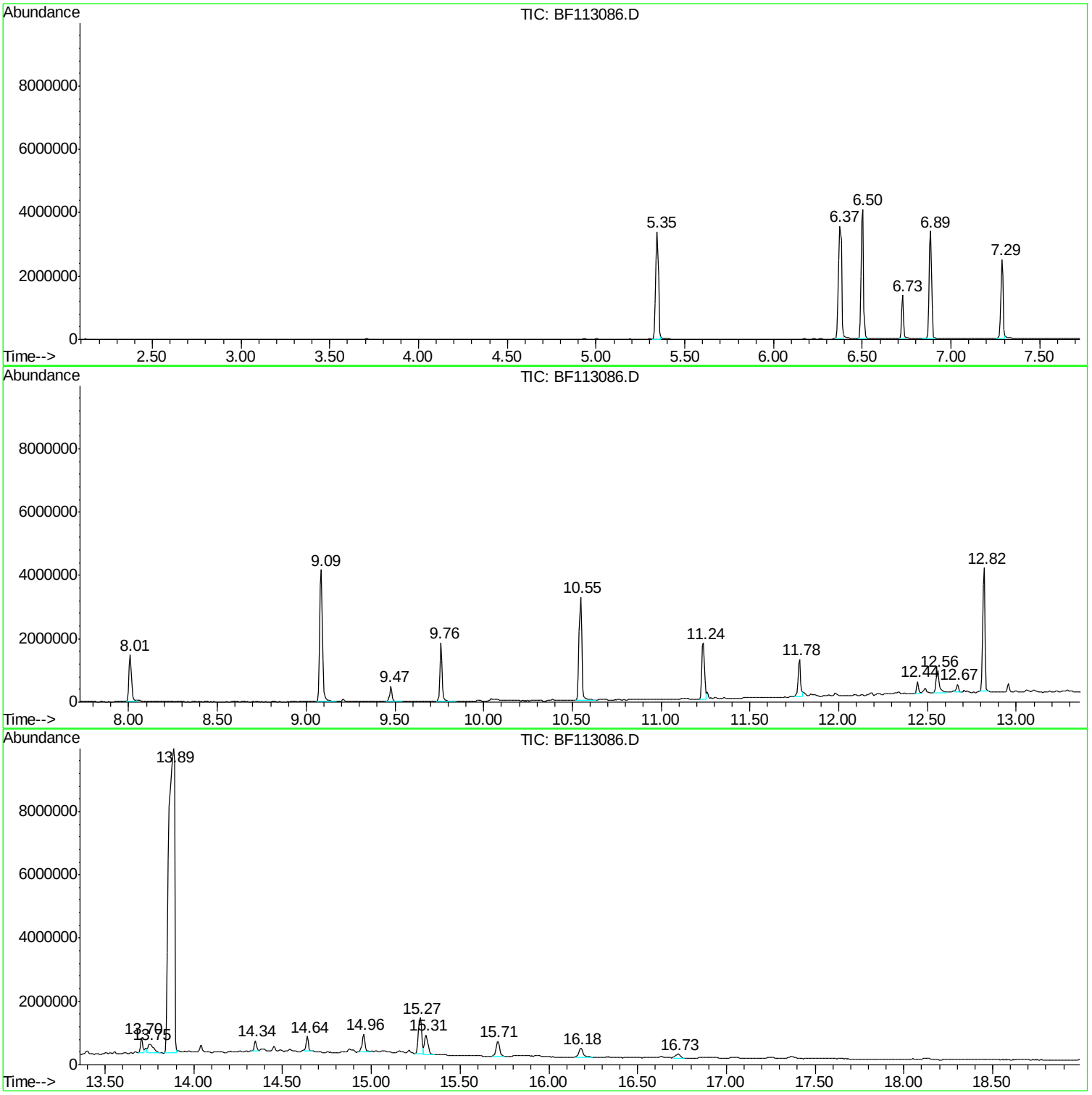
Operator : JU/SJ
Sample : K1933-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-5

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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Instrument : BNA_F
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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

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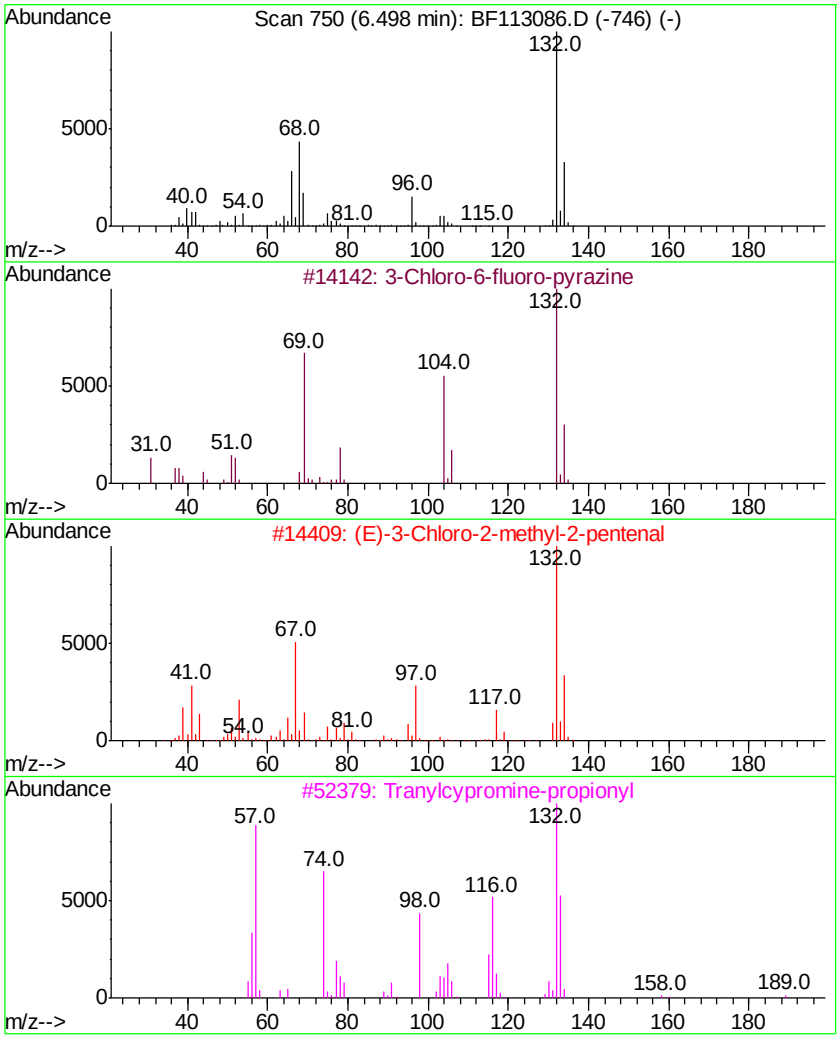
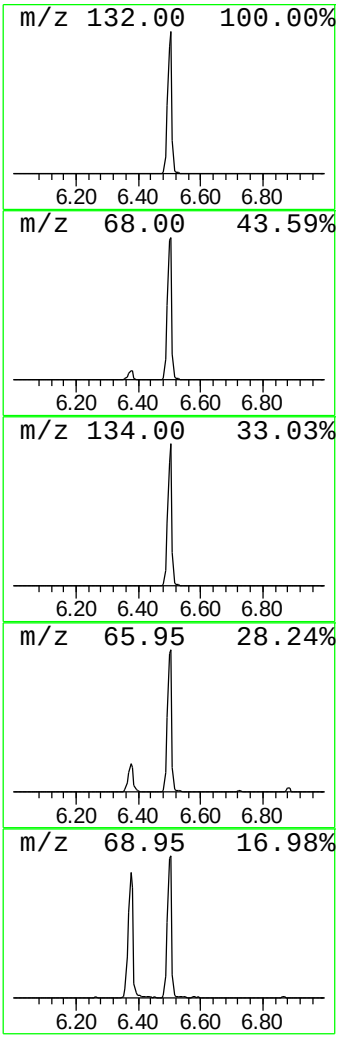
Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	70.98 ng	4008080	1,4-Dichlorobenzene-d4	6.73

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Operator : JU/SJ
Sample : K1933-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-5

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

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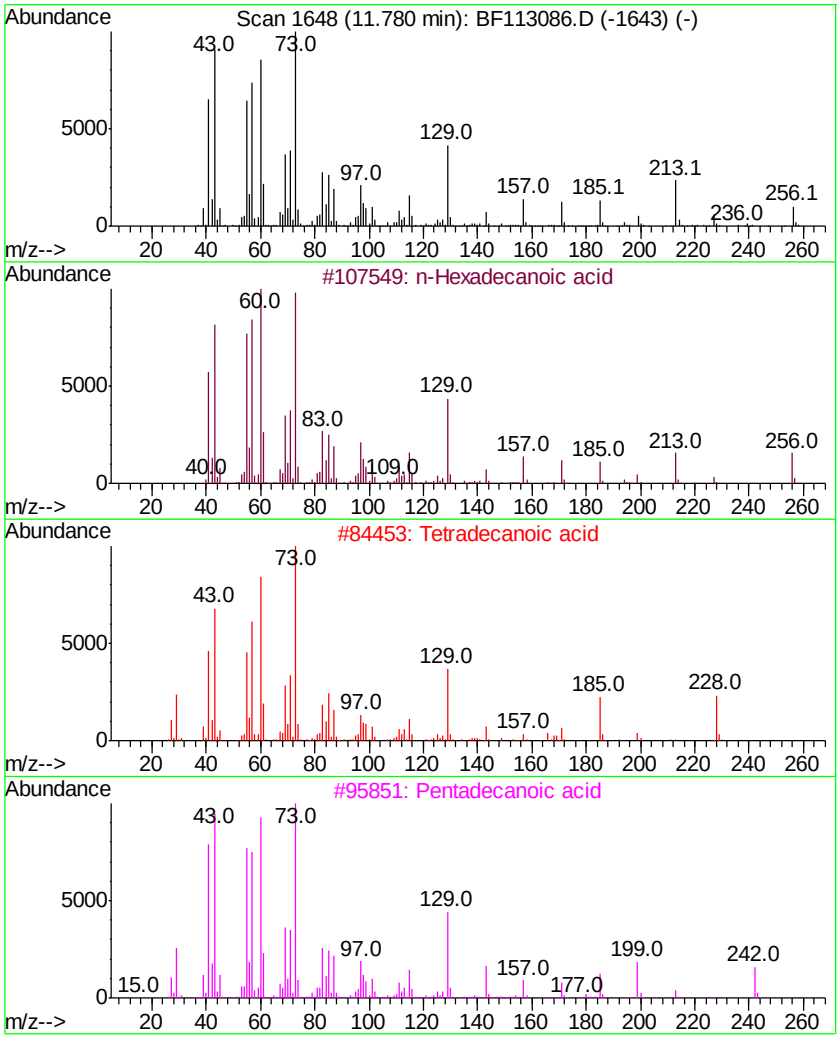
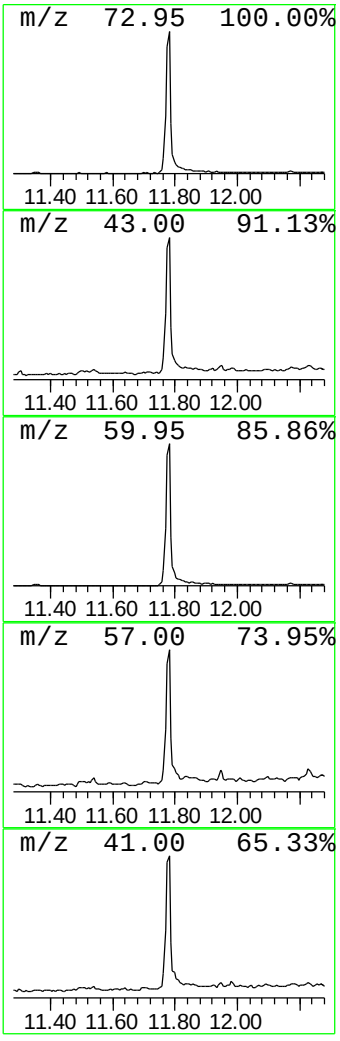
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	14.85 ng	1294230	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	92
5	Undecanoic acid	186	C11H22O2	000112-37-8	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031819\
Data File : BF113086.D
Acq On : 18 Mar 2019 13:21
Operator : JU/SJ
Sample : K1933-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-5

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

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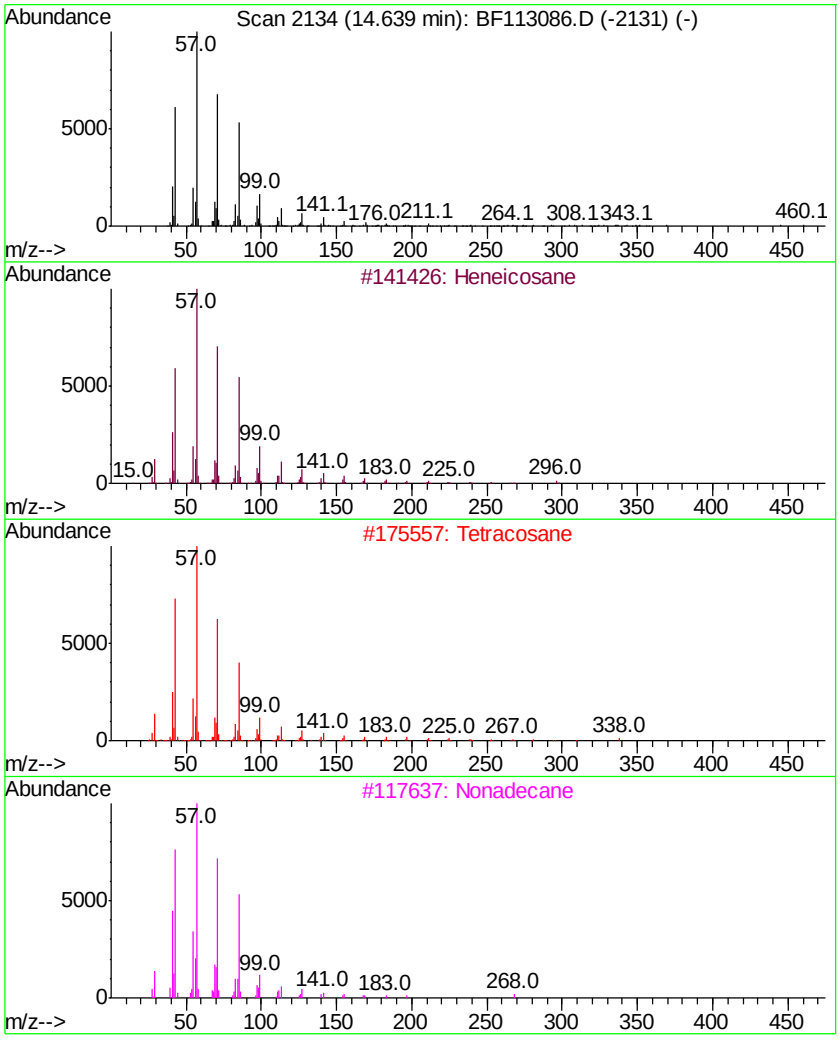
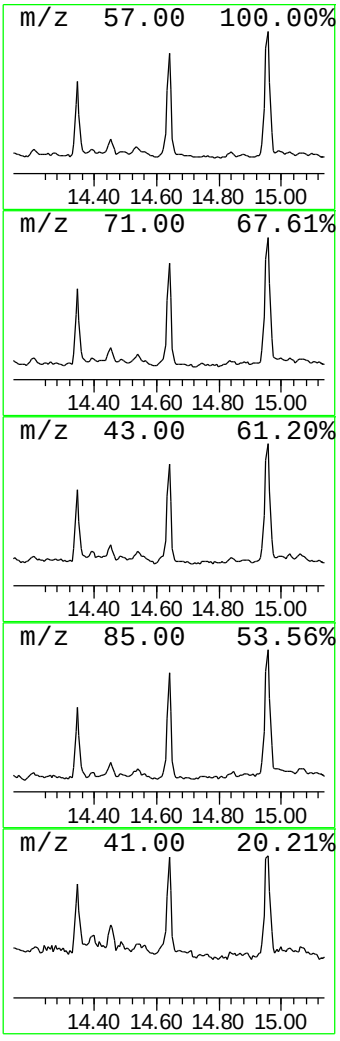
Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	6.58 ng	450117	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Octacosane	394	C28H58	000630-02-4	72
5	Hexatriacontane	507	C36H74	000630-06-8	72





Library Search Compound Report

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Operator : JU/SJ
Sample : K1933-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-5

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

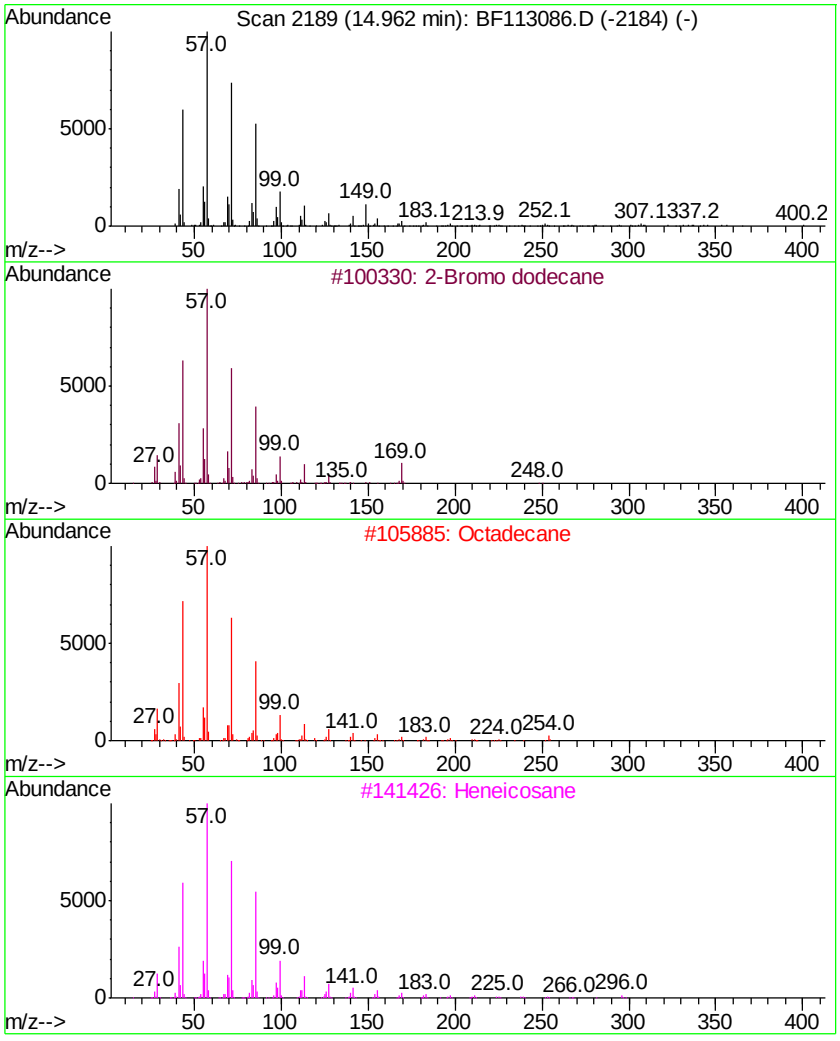
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

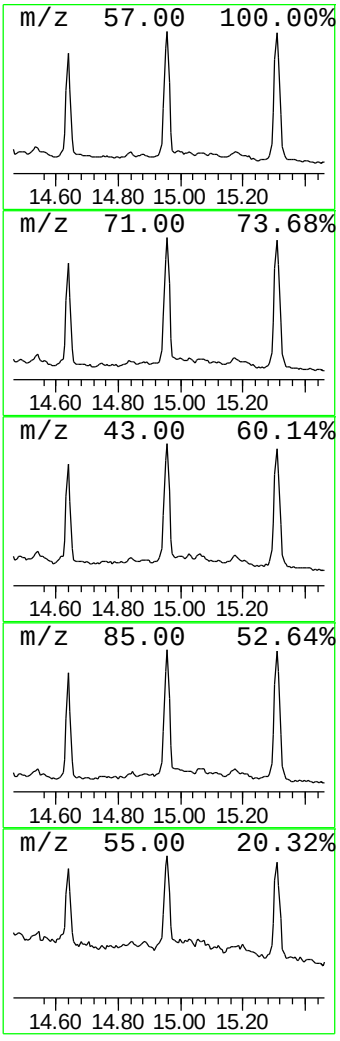
****

Peak Number 5 2-Bromo dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	9.51 ng	650406	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Octadecane	254	C18H38	000593-45-3	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5	Docosane	310	C22H46	000629-97-0	91





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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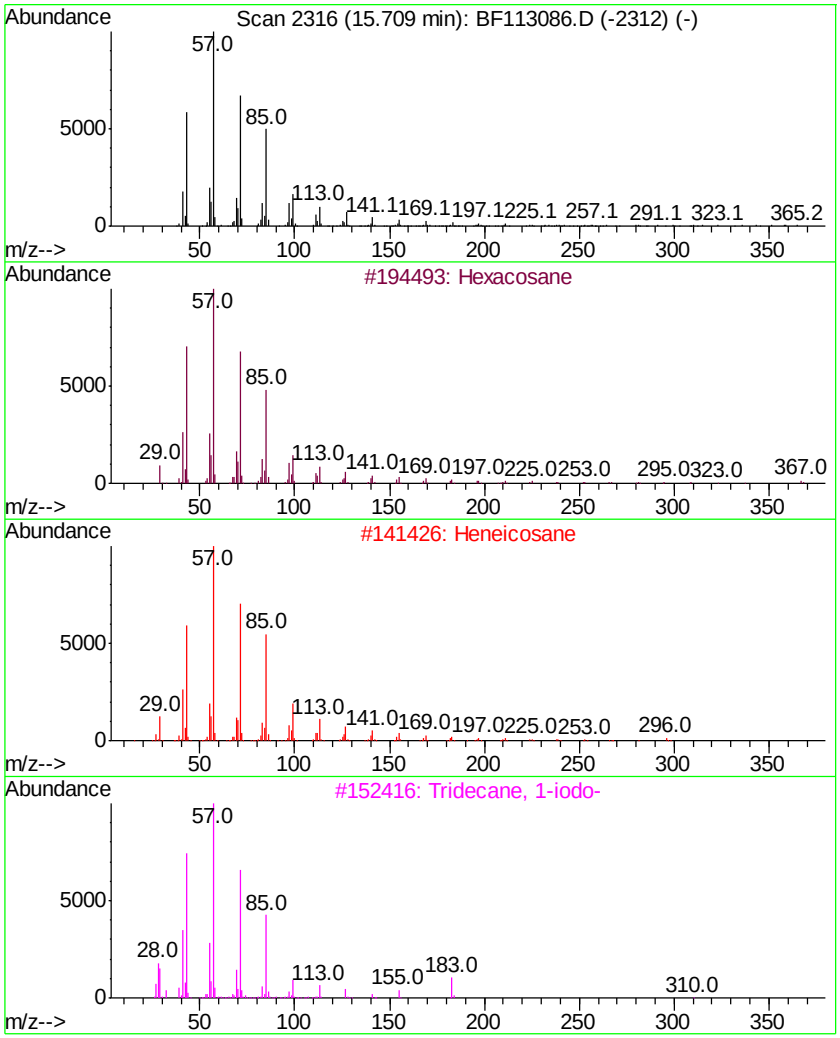
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

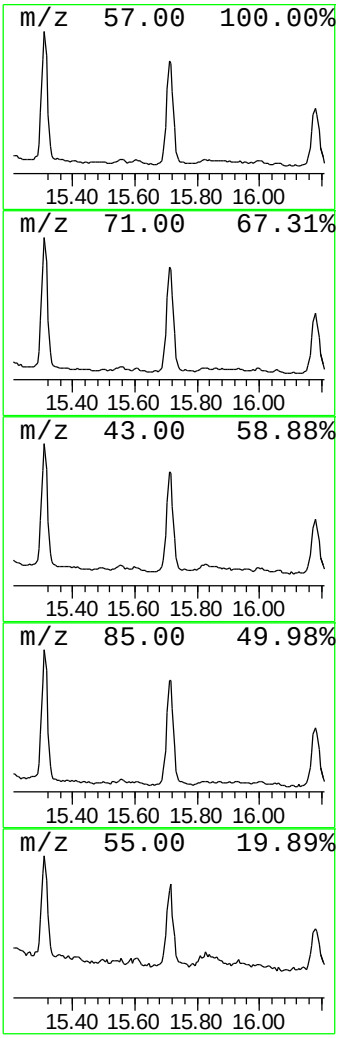
****

Peak Number 6 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	10.47 ng	715646	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





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Misc :
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Instrument : BNA_F
ClientSampleId : S-5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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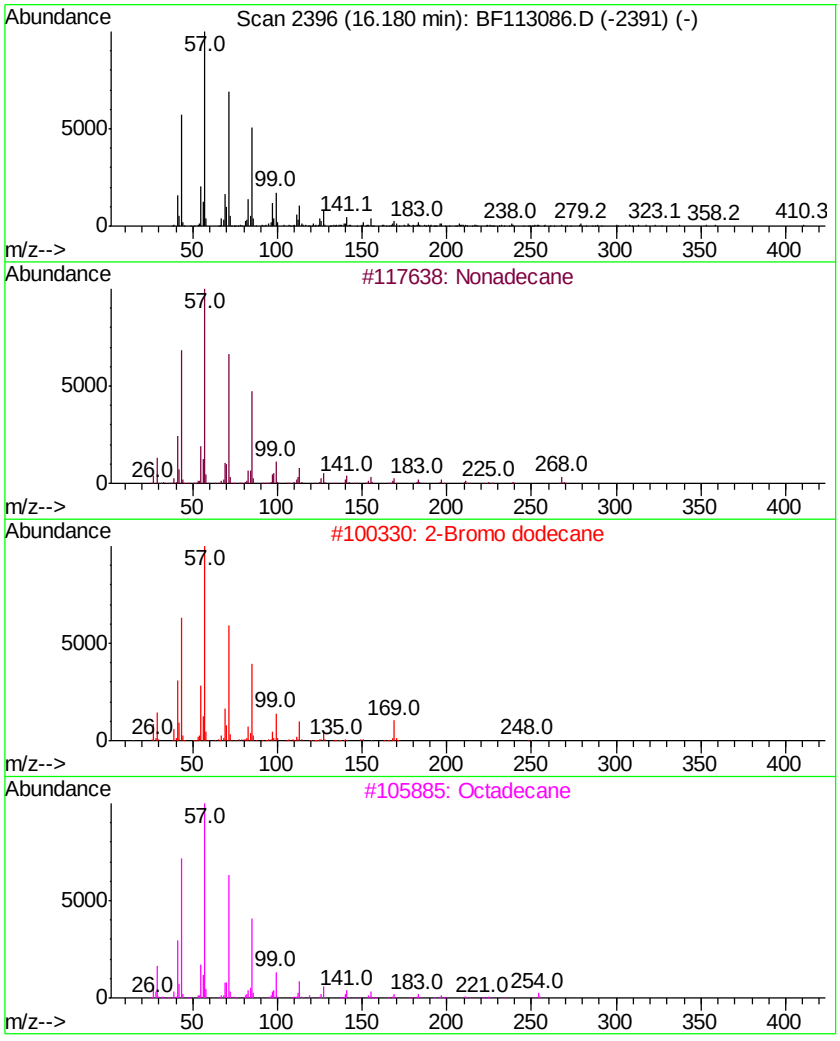
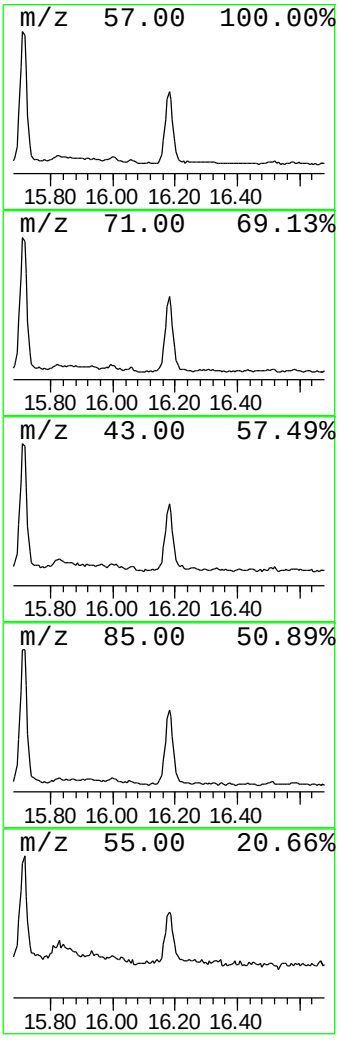
Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	7.74 ng	529154	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3	Octadecane	254	C18H38	000593-45-3	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-5

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

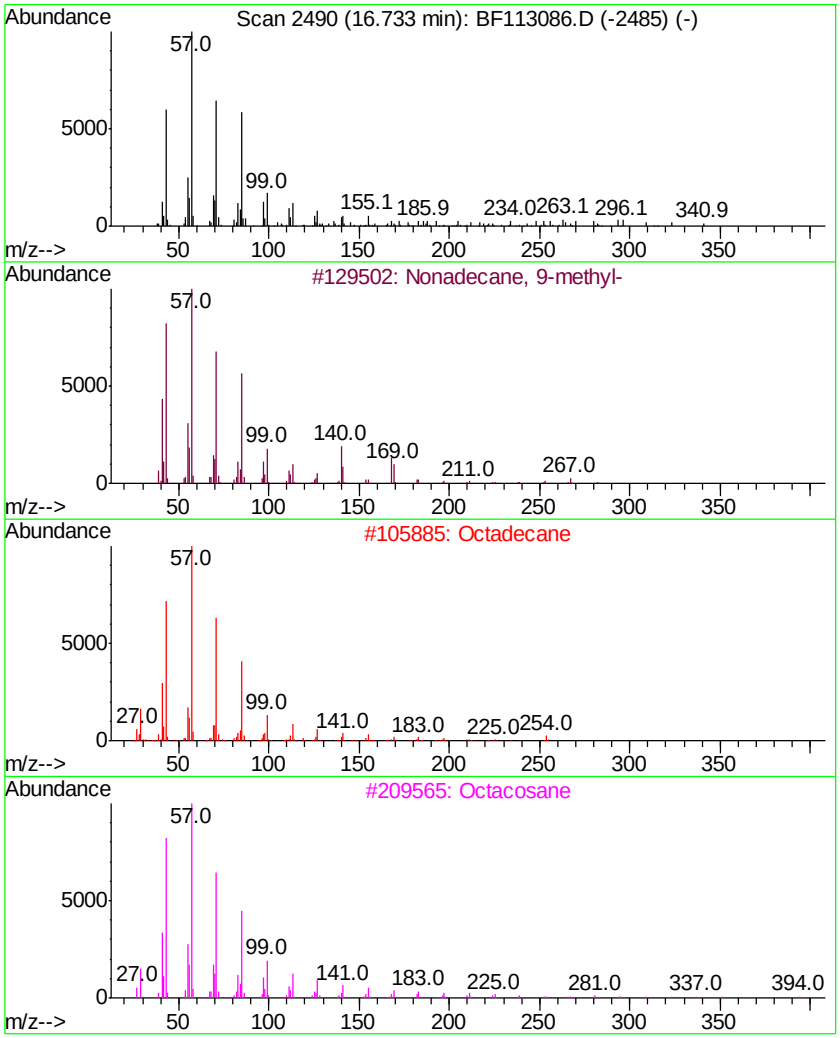
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

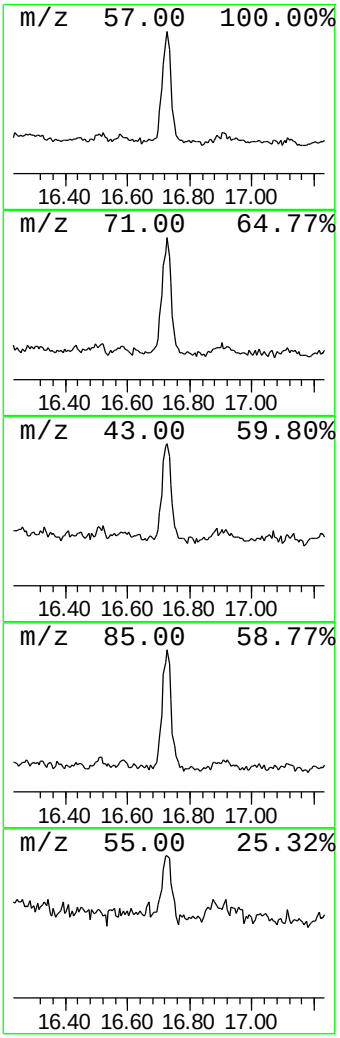
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	3.56 ng	243364	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	94
2	Octadecane	254	C18H38	000593-45-3	93
3	Octacosane	394	C28H58	000630-02-4	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031819\
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.50	6.50	71.0	ng	4008080	1	6.73	1129280	20.0
n-Hexadecanoic acid	11.78	14.9	ng	1294230	4	11.24	1743460	20.0
Heneicosane	14.64	6.6	ng	450117	6	15.27	1367570	20.0
2-Bromo dodecane	14.96	9.5	ng	650406	6	15.27	1367570	20.0
Hexacosane	15.71	10.5	ng	715646	6	15.27	1367570	20.0
Nonadecane	16.18	7.7	ng	529154	6	15.27	1367570	20.0
Nonadecane, 9-met...	16.73	3.6	ng	243364	6	15.27	1367570	20.0