LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112942.D
Acq On : 8 Mar 2019 14:17
Operator : JU/SJ
Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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	4467952	4682100	83.20%	9.816%
2	6.369	722	728	745	rBV	4063636	5036128	89.49%	10.558%
3	6.504	745	751	754	rBV	4616558	4824738	85.73%	10.115%
4	6.728	786	789	793	rBV	1321886	1120740	19.91%	2.350%
5	6.887	812	816	819	rBV	4206101	3753753	66.70%	7.870%
6	7.292	879	885	896	rBV	2811448	3191011	56.70%	6.690%
7	8.010	1003	1007	1014	rBV	1438271	1386130	24.63%	2.906%
8	9.086	1185	1190	1204	rBV	5337725	5443374	96.72%	11.412%
9	9.481	1253	1257	1268	rVB	438539	438657	7.79%	0.920%
10	9.757	1300	1304	1320	rVB	1570894	1608560	28.58%	3.372%
11	10.545	1433	1438	1449	rBV	3589557	3655613	64.96%	7.664%
12	11.233	1552	1555	1570	rVB	1555157	1770652	31.46%	3.712%
13	11.774	1644	1647	1657	rBV2	162963	235502	4.18%	0.494%
14	12.557	1776	1780	1793	rBV	161465	269518	4.79%	0.565%
15	12.821	1820	1825	1828	rBV	5497077	5627797	100.00%	11.798%
16	13.727	1973	1979	1995	rBV2	203829	377166	6.70%	0.791%
17	13.863	1997	2002	2012	rVV	1506597	1678358	29.82%	3.519%
18	14.045	2029	2033	2041	rBV	78273	83950	1.49%	0.176%
19	14.345	2081	2084	2089	rBV	111605	94425	1.68%	0.198%
20	14.639	2130	2134	2140	rBV	152487	149964	2.66%	0.314%
21	14.710	2142	2146	2150	rVB	116805	112825	2.00%	0.237%
22	14.957	2184	2188	2195	rVB	155923	170593	3.03%	0.358%
23	15.262	2235	2240	2245	rBV	878579	1234809	21.94%	2.589%
24	15.310	2245	2248	2255	rVB	188539	260630	4.63%	0.546%
25	15.715	2312	2317	2324	rVB	160399	227490	4.04%	0.477%
26	16.180	2391	2396	2404	rVB2	102316	185978	3.30%	0.390%
27	16.727	2484	2489	2496	rVB3	39550	78879	1.40%	0.165%

Sum of corrected areas: 47699340

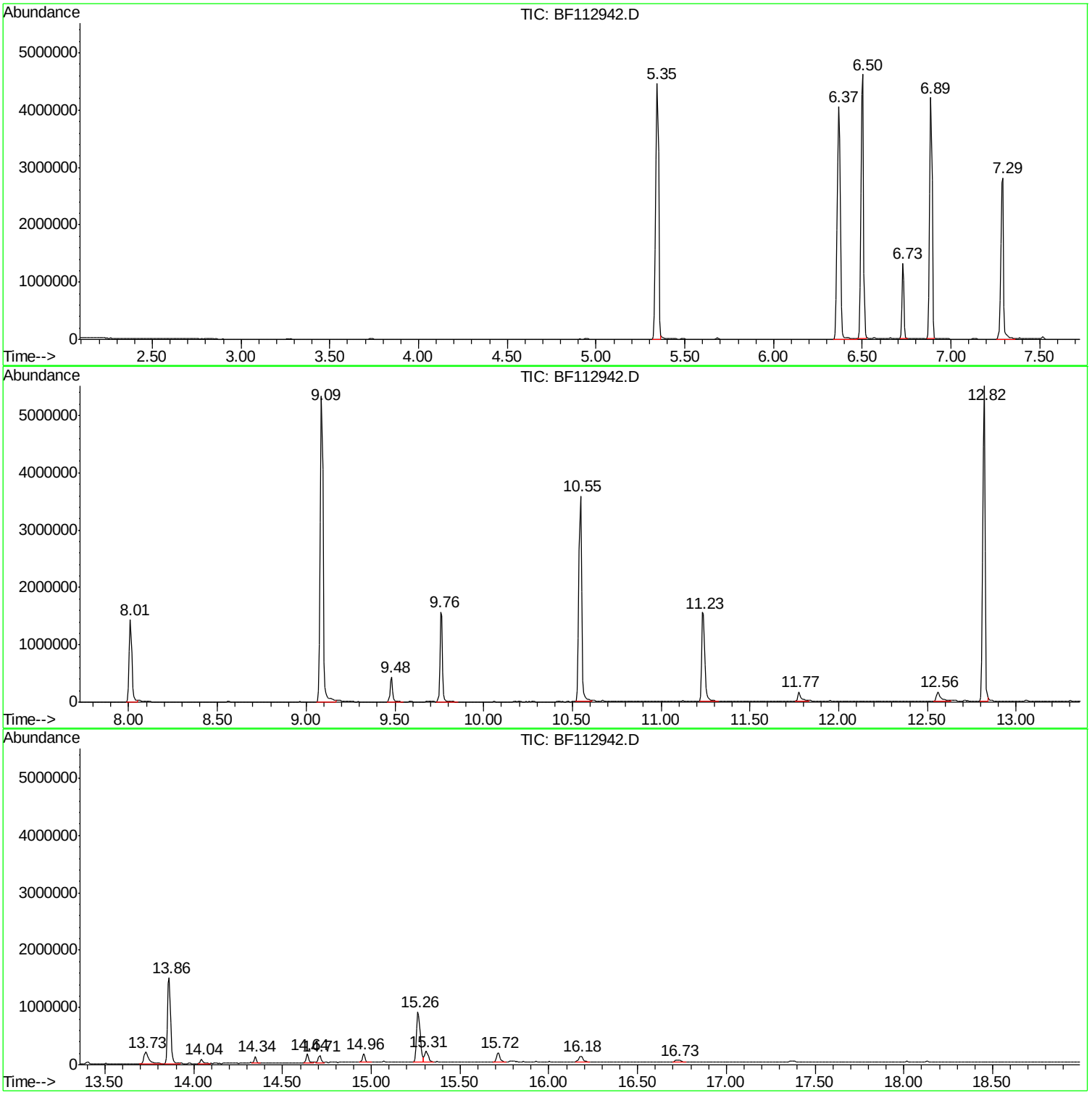
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112942.D
Acq On : 8 Mar 2019 14:17
Operator : JU/SJ
Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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\BF030819\
Data File : BF112942.D
Acq On : 8 Mar 2019 14:17
Operator : JU/SJ
Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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

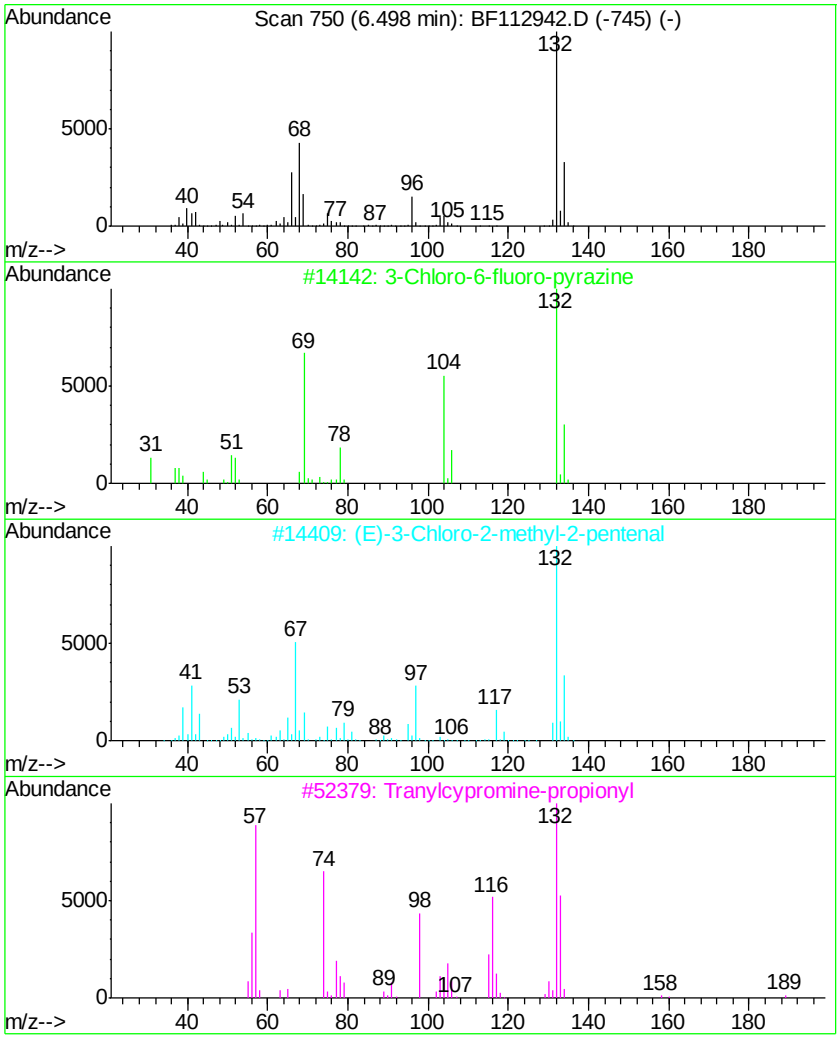
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

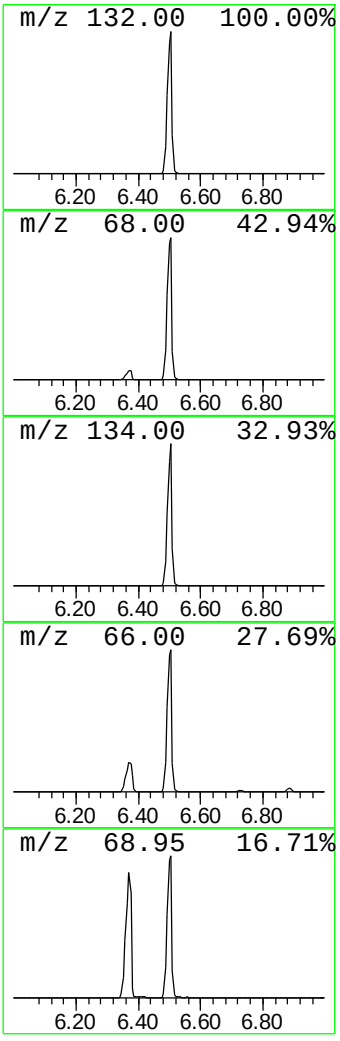
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	86.10 ng	4824740	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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

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Data File : BF112942.D
Acq On : 8 Mar 2019 14:17
Operator : JU/SJ
Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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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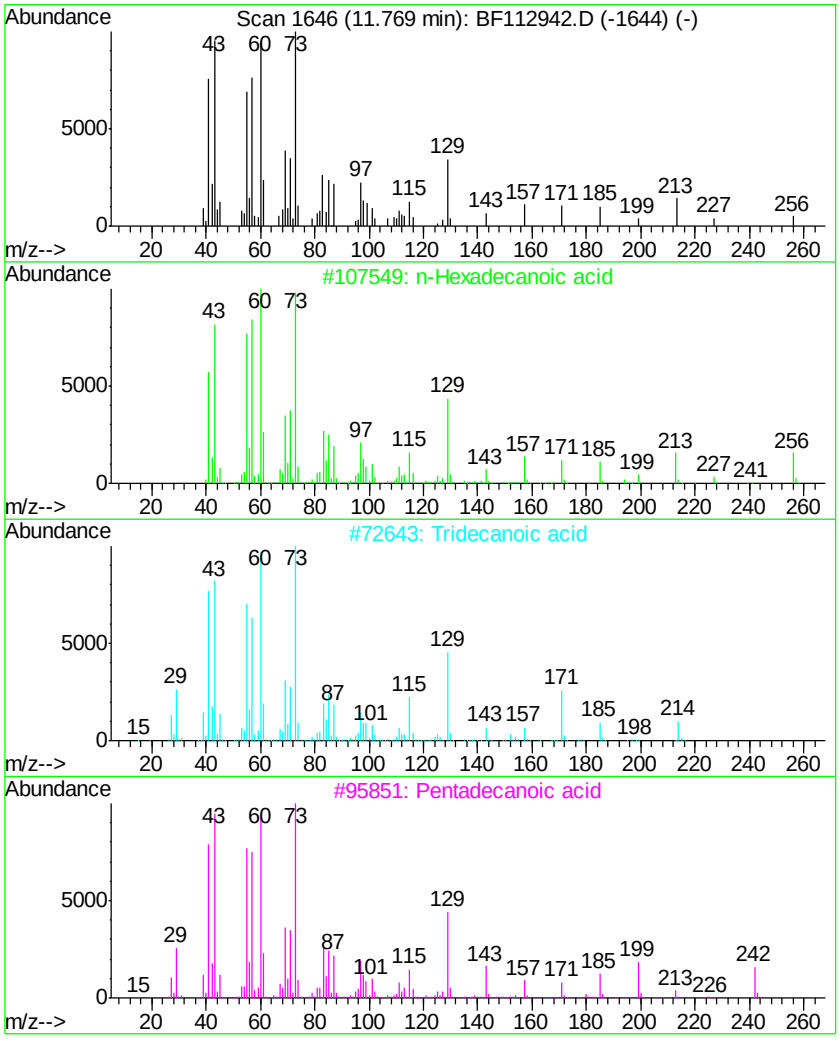
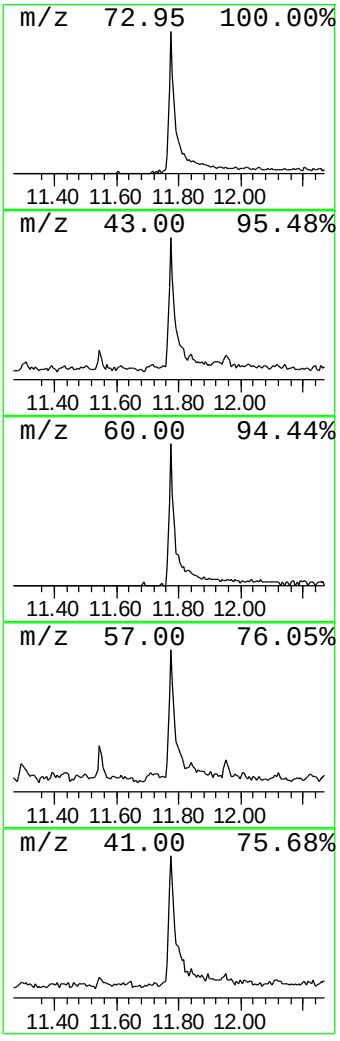
Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.66 ng	235502	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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112942.D
Acq On : 8 Mar 2019 14:17
Operator : JU/SJ
Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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

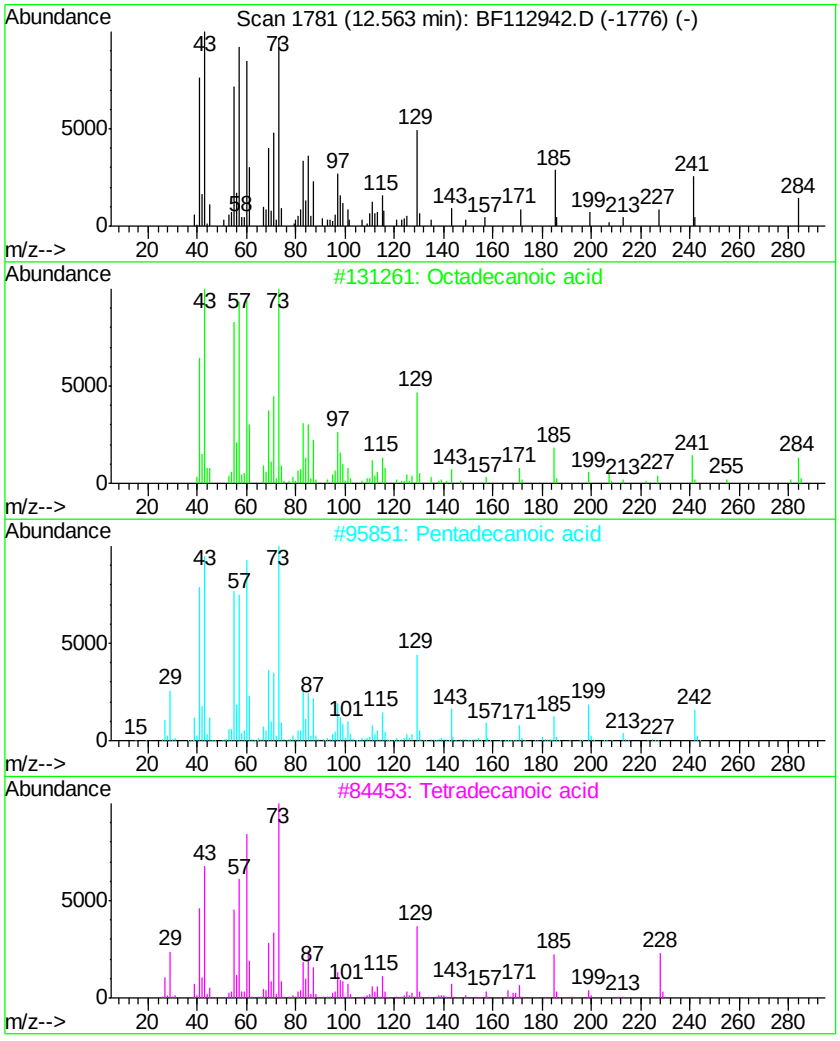
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

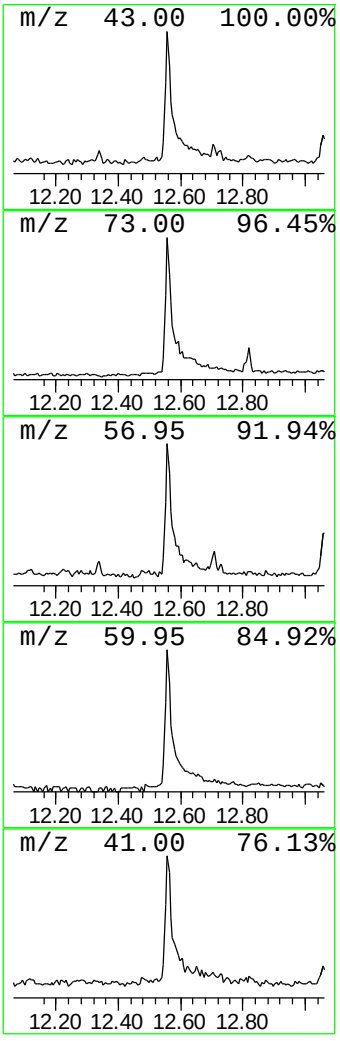
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	3.21 ng	269518	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	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112942.D
Acq On : 8 Mar 2019 14:17
Operator : JU/SJ
Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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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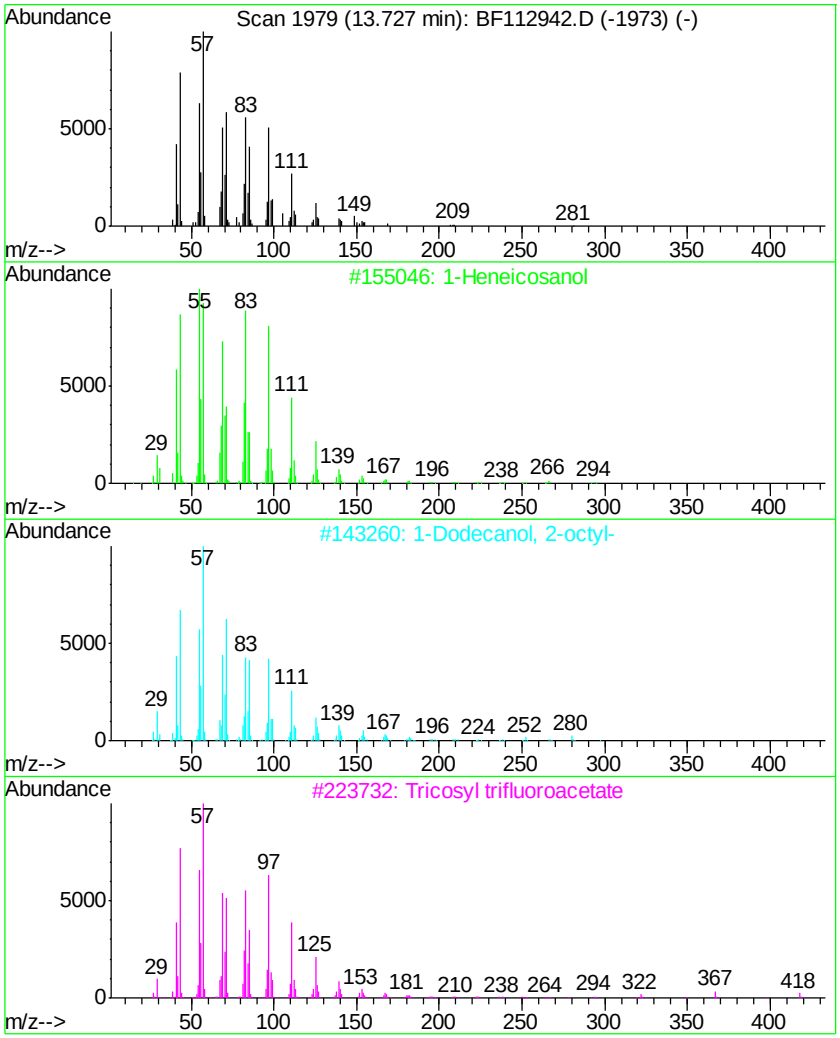
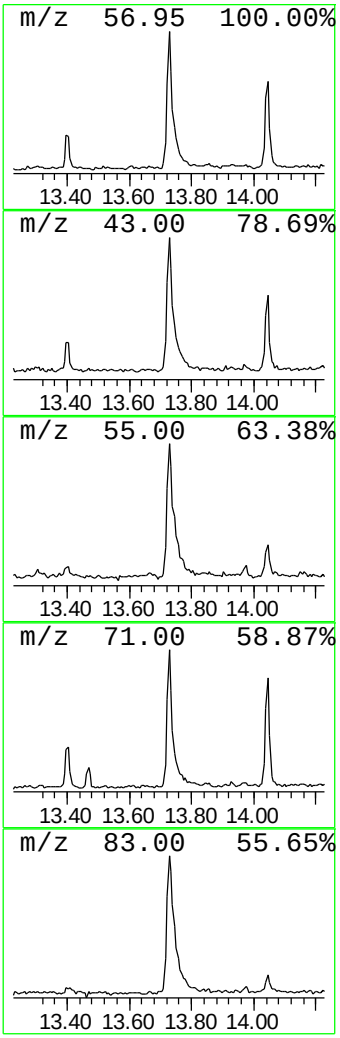
Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.49 ng	377166	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	92
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112942.D
Acq On : 8 Mar 2019 14:17
Operator : JU/SJ
Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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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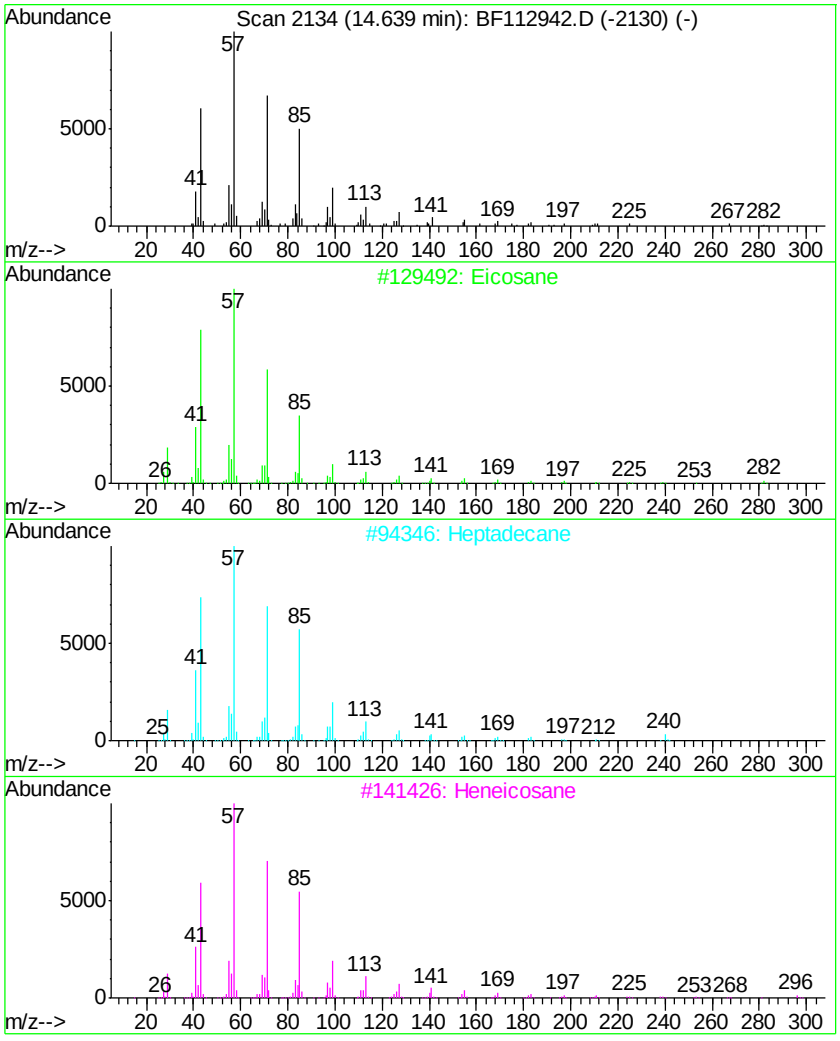
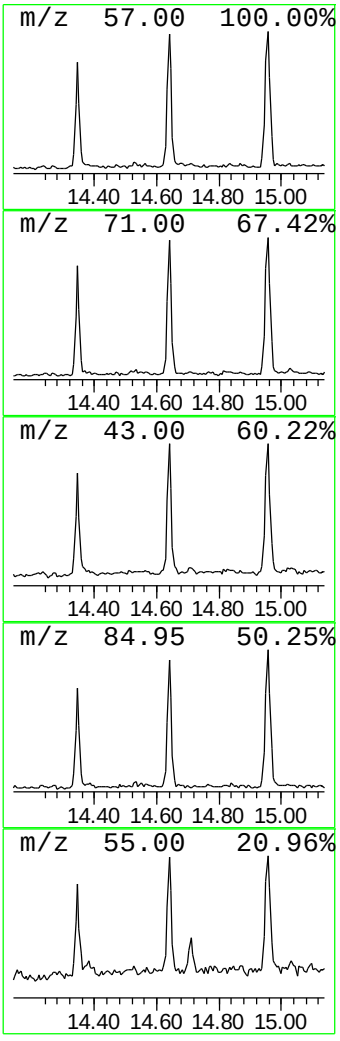
Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.43 ng	149964	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Hexacosane	366	C26H54	000630-01-3	87





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Sample : K1807-29
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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

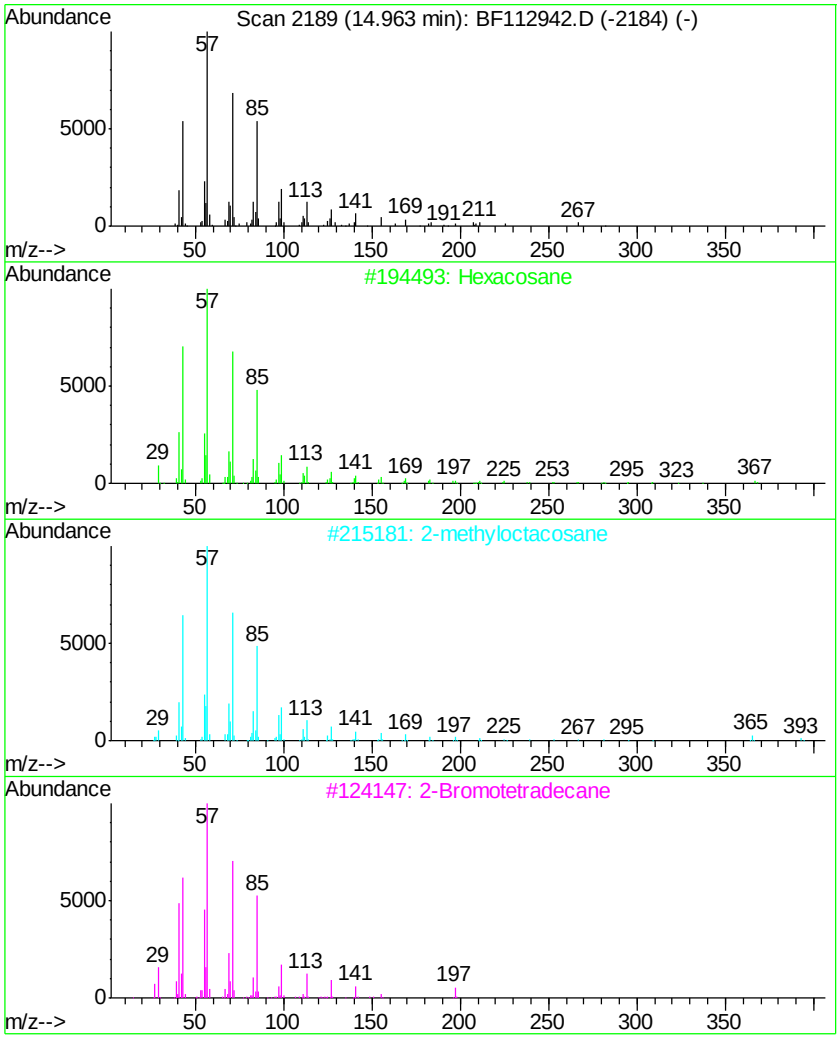
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

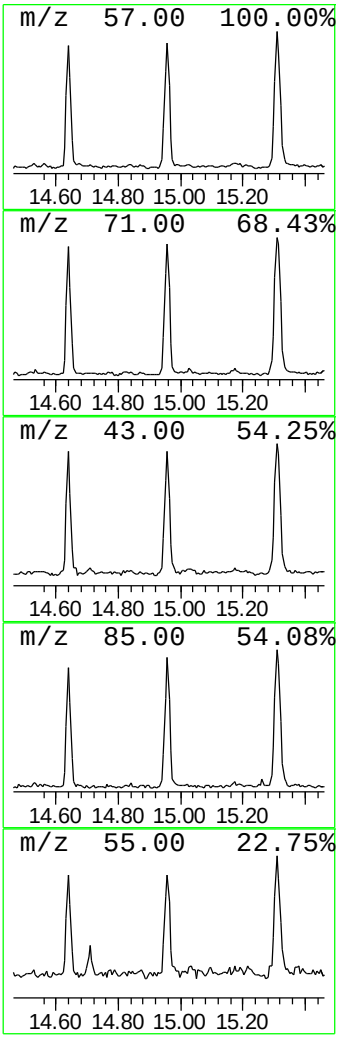
****

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.76 ng	170593	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-14

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

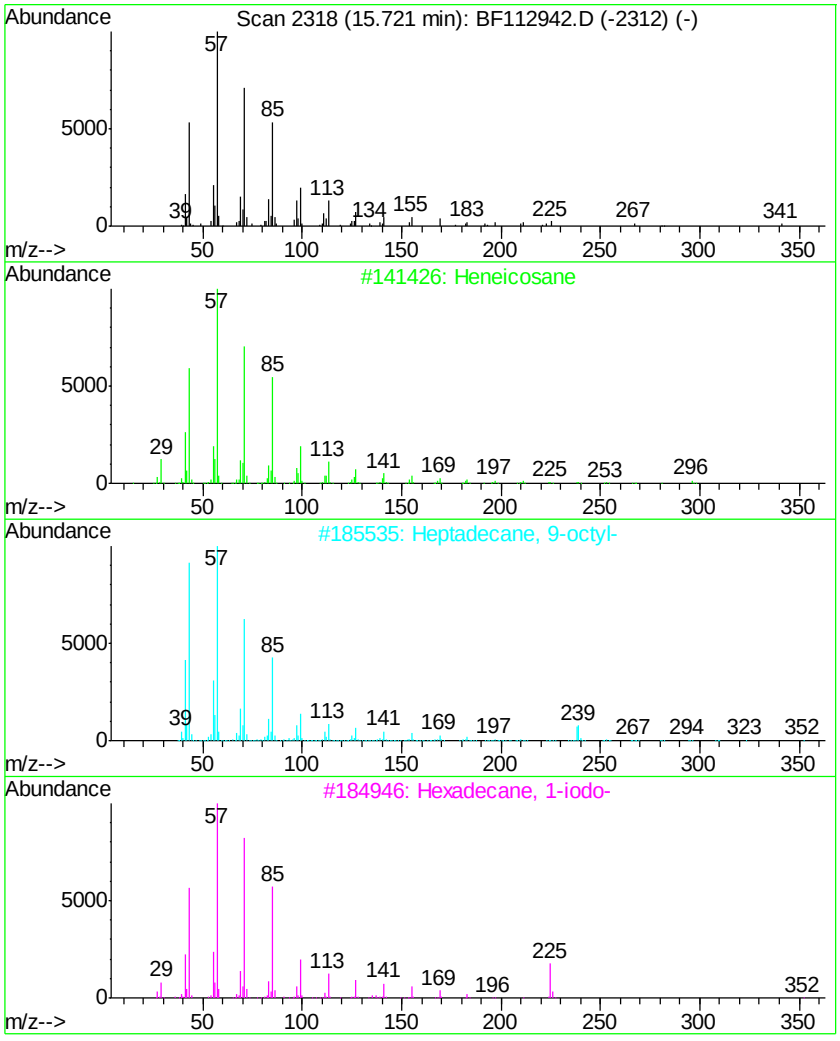
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

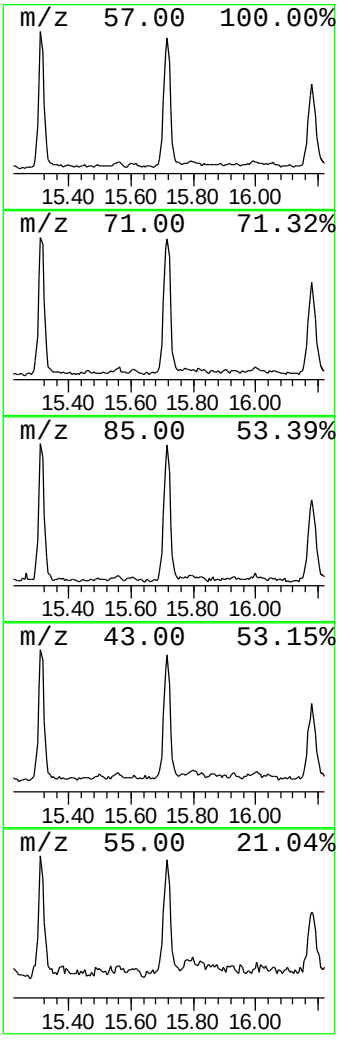
****

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.68 ng	227490	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
4	Octadecane	254	C18H38	000593-45-3	87
5	Tetracosane	338	C24H50	000646-31-1	86





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-14

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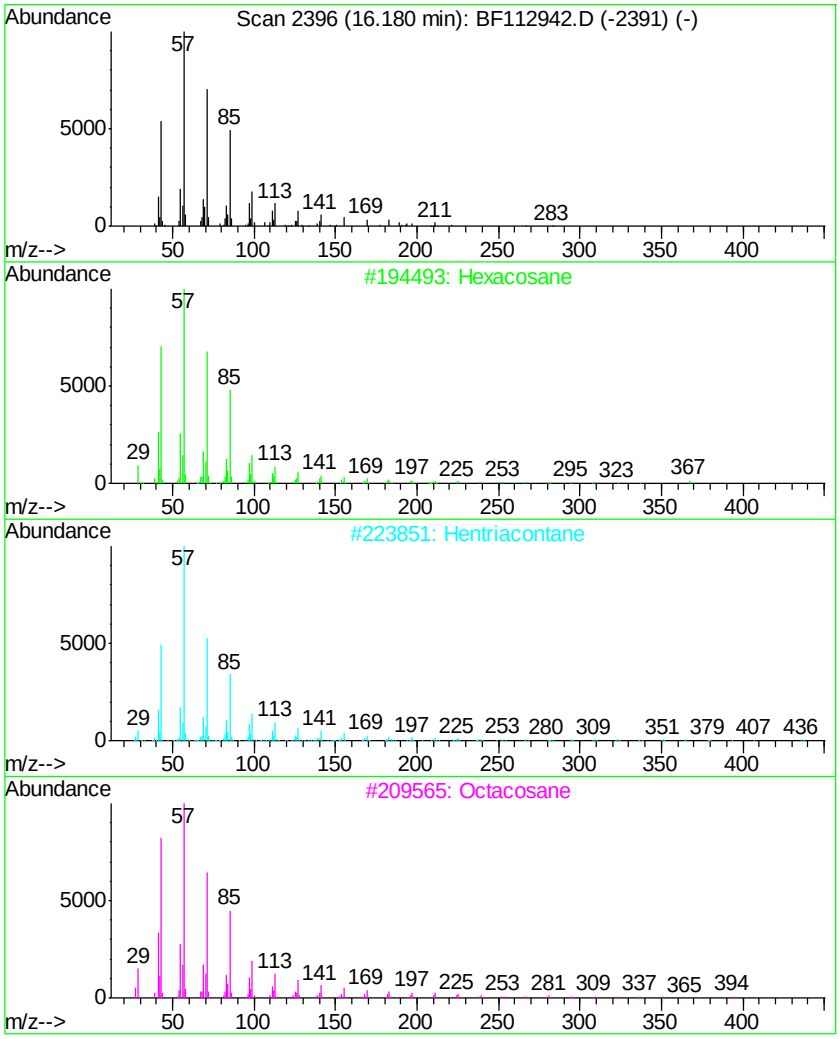
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

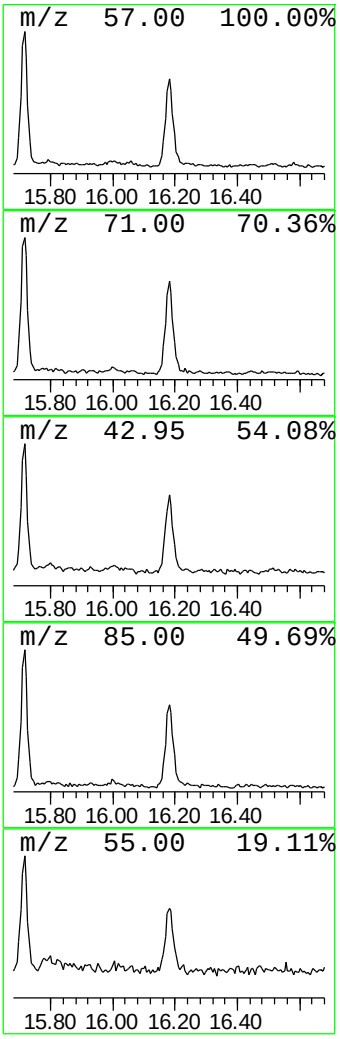
****

Peak Number 9 unknown16.18 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	3.01 ng	185978	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.50	6.50	86.1	ng	4824740	1	6.73	1120740	20.0
n-Hexadecanoic acid	11.77	2.7	ng	235502	4	11.23	1770650	20.0
Octadecanoic acid	12.56	3.2	ng	269518	5	13.86	1678360	20.0
1-Heneicosanol	13.73	4.5	ng	377166	5	13.86	1678360	20.0
Eicosane	14.64	2.4	ng	149964	6	15.26	1234810	20.0
Hexacosane	14.96	2.8	ng	170593	6	15.26	1234810	20.0
Heneicosane	15.72	3.7	ng	227490	6	15.26	1234810	20.0
unknown16.18	16.18	3.0	ng	185978	6	15.26	1234810	20.0