LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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	5.340	549	553	568	rBV	1865051	1731482	91.86%	7.174%
2	6.363	723	727	746	rBV	1920698	1735777	92.09%	7.192%
3	6.498	746	750	754	rBV	2121148	1798052	95.39%	7.450%
4	6.734	786	790	793	rBV	1137435	1009939	53.58%	4.185%
5	6.887	812	816	820	rBV	1685002	1357600	72.02%	5.625%
6	7.287	880	884	896	rBV	1081544	1011747	53.68%	4.192%
7	8.010	1004	1007	1014	rBV	1136237	1175916	62.39%	4.872%
8	9.086	1186	1190	1204	rBV	1829870	1711910	90.82%	7.093%
9	9.481	1253	1257	1263	rVB	92583	86485	4.59%	0.358%
10	9.763	1301	1305	1309	rBV	1340284	1243751	65.98%	5.153%
11	9.969	1335	1340	1345	rBV2	21726	30660	1.63%	0.127%
12	10.304	1395	1397	1404	rVB2	21042	22683	1.20%	0.094%
13	10.545	1434	1438	1449	rBV	1153482	1203327	63.84%	4.986%
14	10.916	1497	1501	1505	rBV4	19694	27982	1.48%	0.116%
15	11.045	1520	1523	1528	rVB	20512	23426	1.24%	0.097%
16	11.210	1546	1551	1552	rBV3	14519	21839	1.16%	0.090%
17	11.239	1552	1556	1558	rVV	1479813	1308352	69.41%	5.421%
18	11.263	1558	1560	1566	rVV	299370	299413	15.88%	1.241%
19	11.310	1566	1568	1573	rVB	66456	65197	3.46%	0.270%
20	11.469	1590	1595	1597	rBV3	24026	28145	1.49%	0.117%
21	11.645	1619	1625	1631	rVB9	10715	21828	1.16%	0.090%
22	11.704	1631	1635	1638	rBV5	14129	24178	1.28%	0.100%
23	11.739	1638	1641	1643	rBV	47615	41223	2.19%	0.171%
24	11.774	1643	1647	1652	rBV2	354715	384373	20.39%	1.593%
25	11.851	1657	1660	1662	rBV	49741	53452	2.84%	0.221%
26	12.033	1688	1691	1693	rBV	32282	31449	1.67%	0.130%
27	12.051	1693	1694	1698	rVB2	27604	23763	1.26%	0.098%
28	12.180	1714	1716	1719	rBV3	21430	21562	1.14%	0.089%
29	12.286	1731	1734	1737	rBV2	40895	47709	2.53%	0.198%
30	12.369	1745	1748	1752	rVB3	30344	34390	1.82%	0.142%
31	12.445	1757	1761	1765	rBV	385062	365644	19.40%	1.515%
32	12.492	1765	1769	1775	rVB9	22183	49100	2.60%	0.203%
33	12.557	1777	1780	1785	rBV2	133495	167592	8.89%	0.694%
34	12.669	1794	1799	1806	rBV2	318324	378881	20.10%	1.570%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

35	12.792	1817	1820	1821	rBV	34844	30480	1.62%	0.126%
36	12.816	1821	1824	1831	rVB	2121364	1884917	100.00%	7.810%
37	13.039	1861	1862	1864	rBV2	22262	21230	1.13%	0.088%
38	13.104	1870	1873	1876	rVB2	46424	43308	2.30%	0.179%
39	13.504	1938	1941	1947	rBV	51160	86410	4.58%	0.358%
40	13.727	1976	1979	1985	rVB	212128	233691	12.40%	0.968%
41	13.863	1997	2002	2005	rBV	1694094	1733942	91.99%	7.184%
42	14.045	2031	2033	2037	rVB2	120142	99858	5.30%	0.414%
43	14.351	2082	2085	2097	rBV4	203477	415421	22.04%	1.721%
44	14.645	2132	2135	2140	rVB	219773	220874	11.72%	0.915%
45	14.774	2155	2157	2161	rVB	156231	150944	8.01%	0.625%
46	14.963	2186	2189	2191	rBV	205179	216356	11.48%	0.896%
47	15.268	2237	2241	2245	rBV	848771	974832	51.72%	4.039%
48	15.315	2246	2249	2253	rVB2	196488	257154	13.64%	1.065%
49	15.721	2315	2318	2323	rVB	171237	226501	12.02%	0.938%

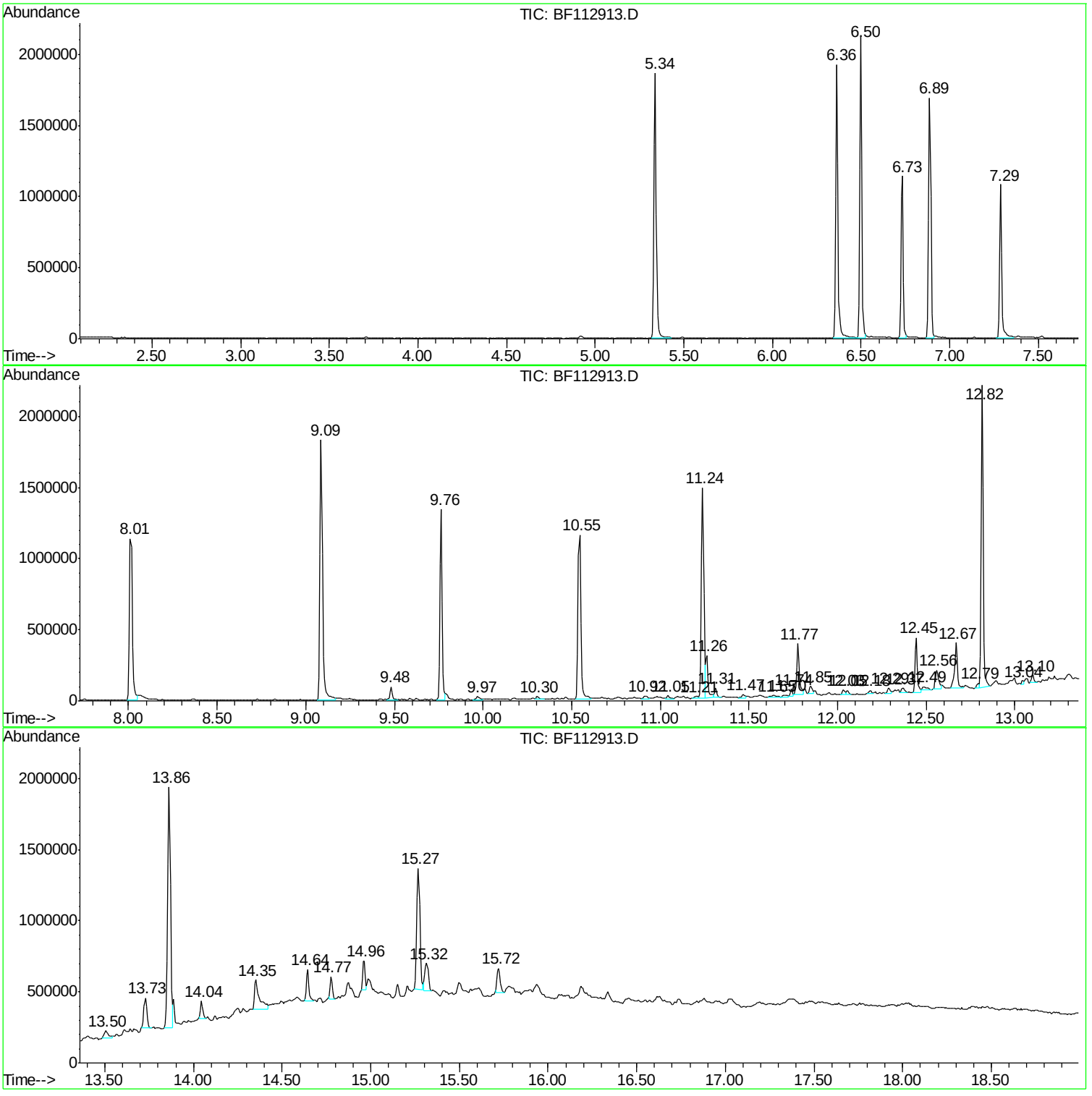
Sum of corrected areas: 24134745

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-027-SW024-022719

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

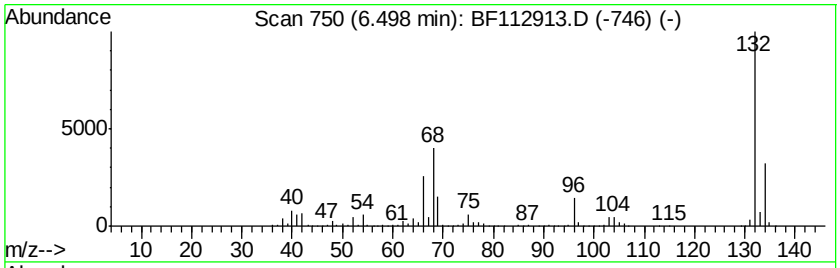
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

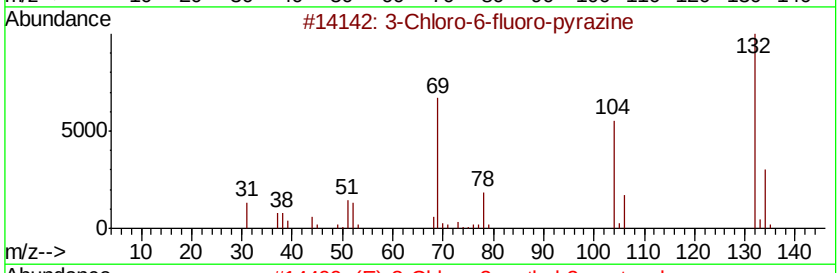
****

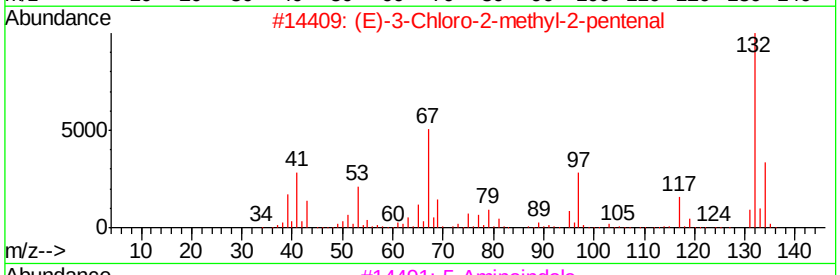
Peak Number 1 unknown6.50 Concentration Rank 1

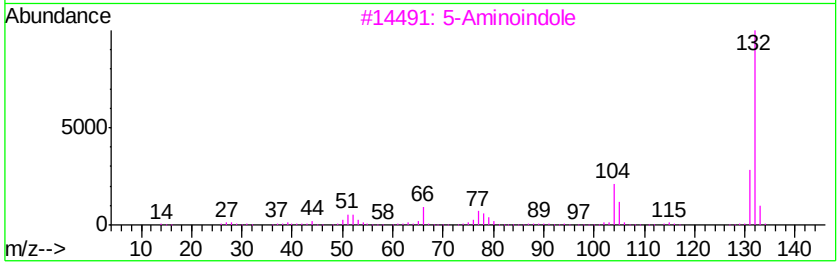
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	35.61 ng	1798050	1,4-Dichlorobenzene-d4	6.73

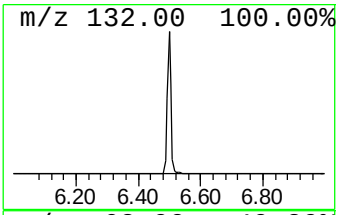
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9

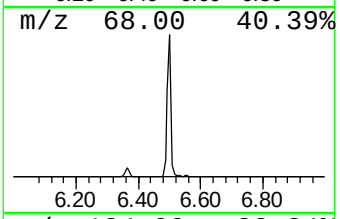


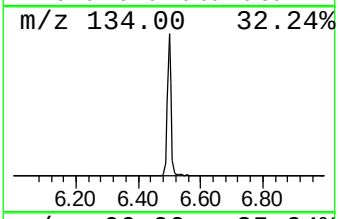


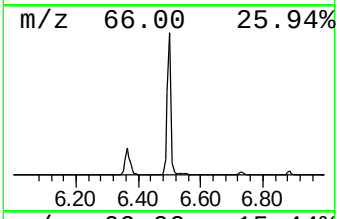


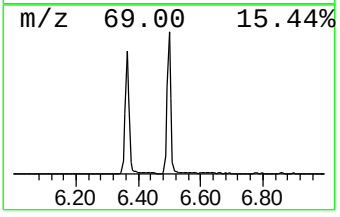












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

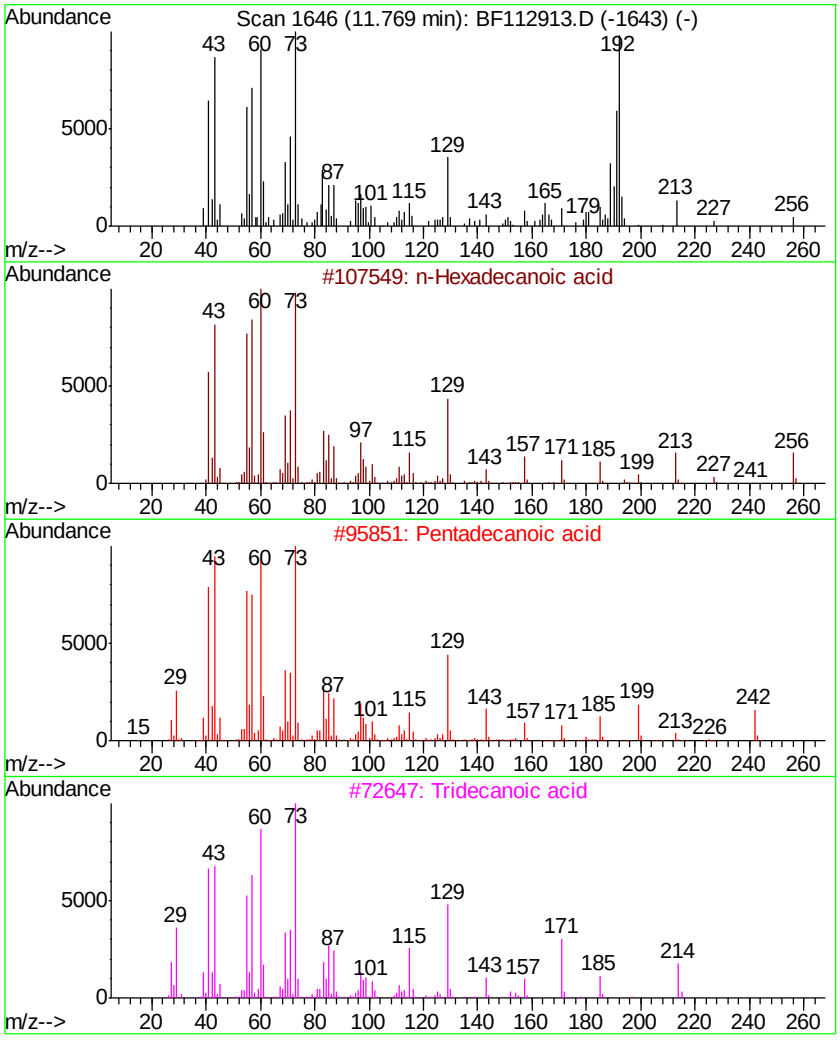
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

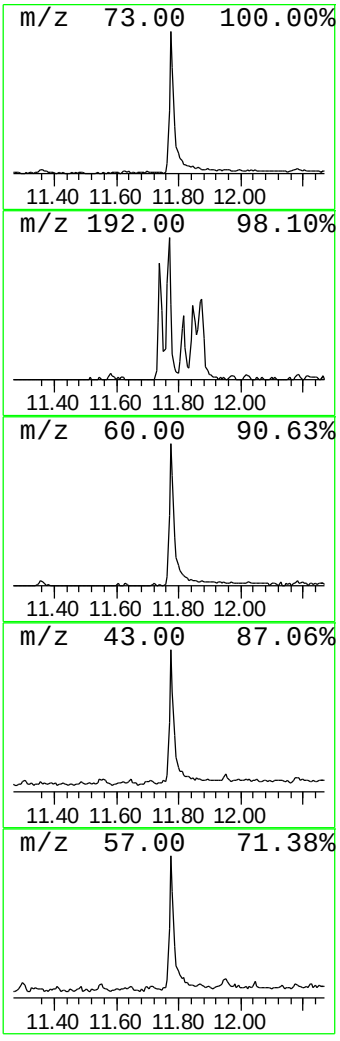
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	5.88 ng	384373	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

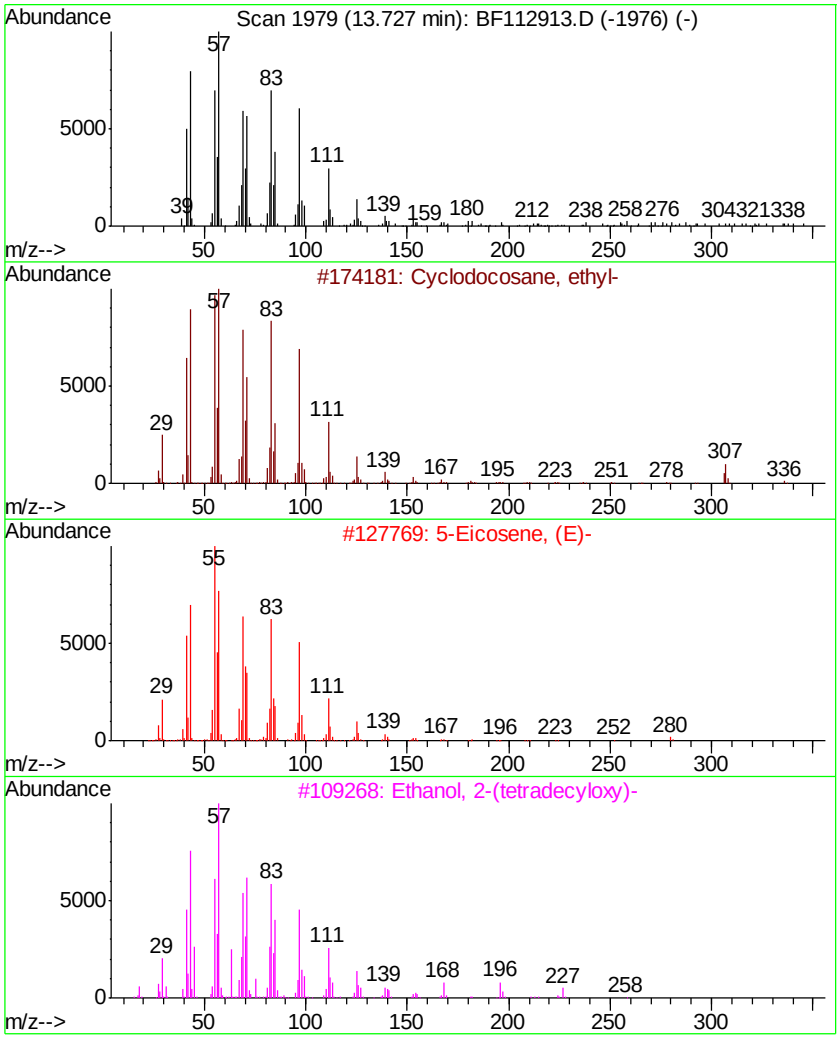
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

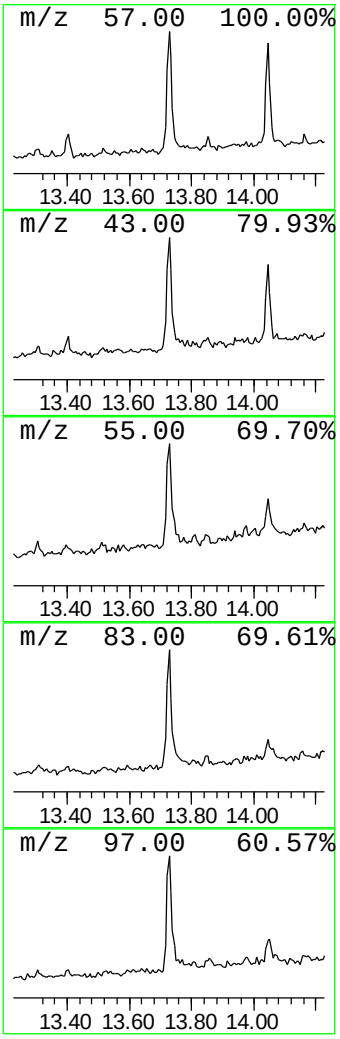
****

Peak Number 4 Cyclodocosane, ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.70 ng	233691	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	92
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

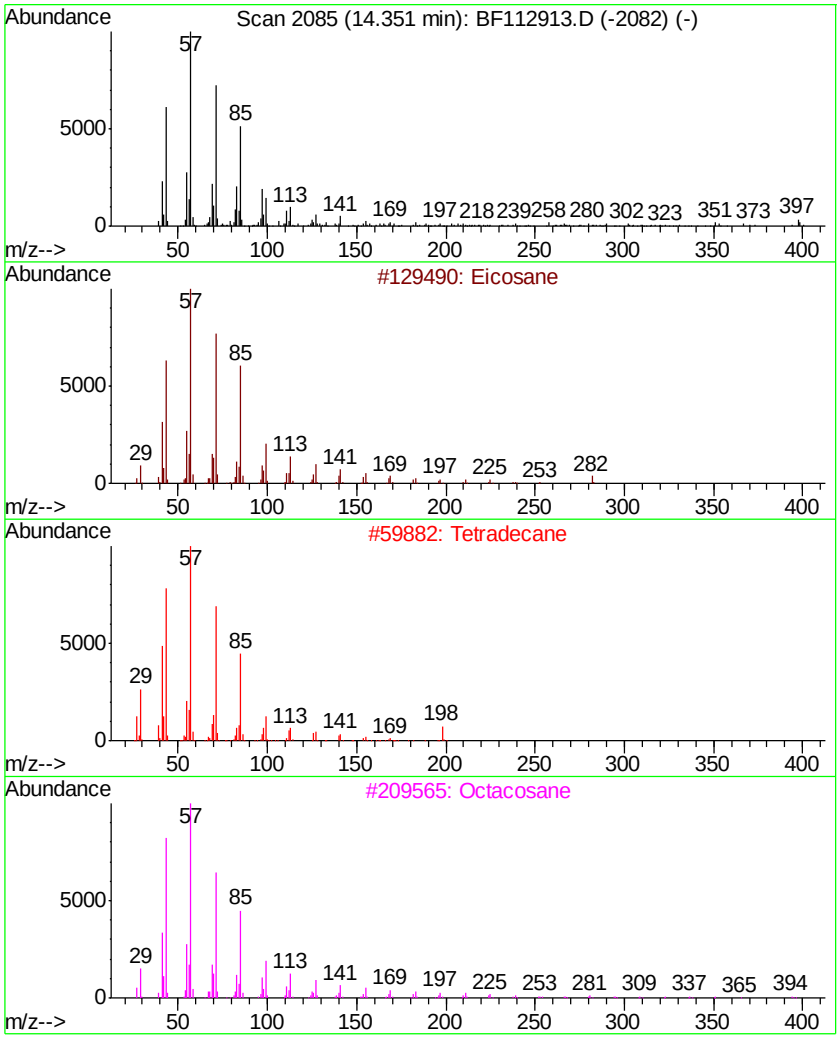
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

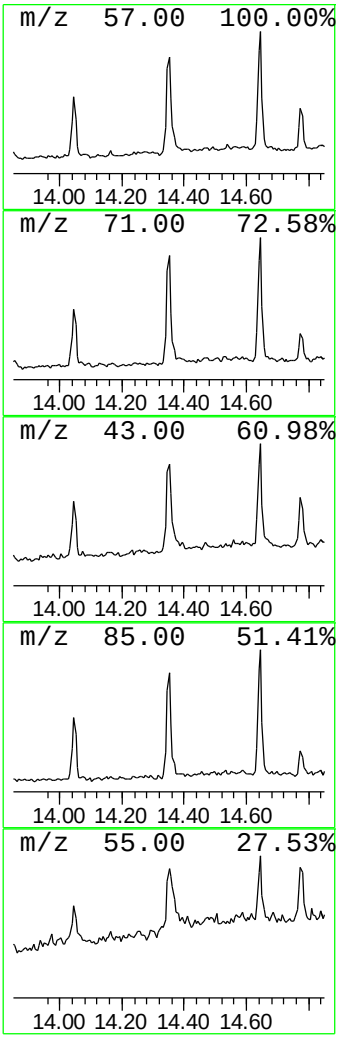
****

Peak Number 5 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	4.79 ng	415421	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Tetradecane	198	C14H30	000629-59-4	89
3	Octacosane	394	C28H58	000630-02-4	87
4	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	87
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

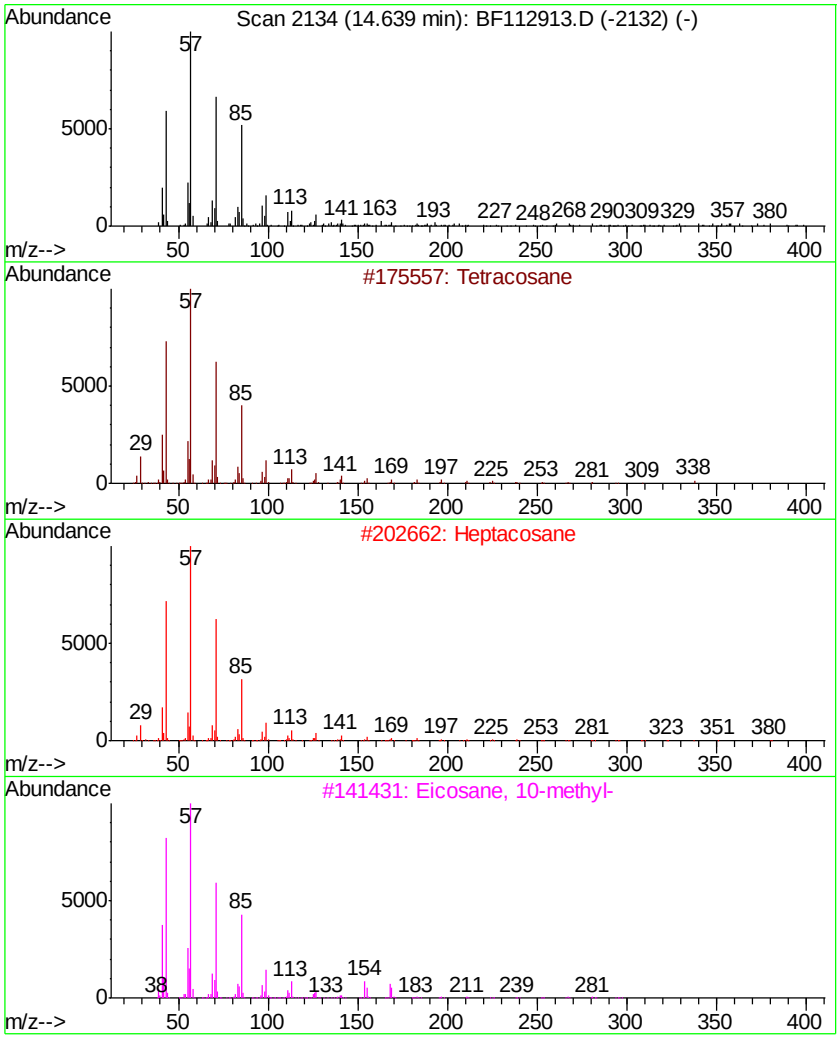
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

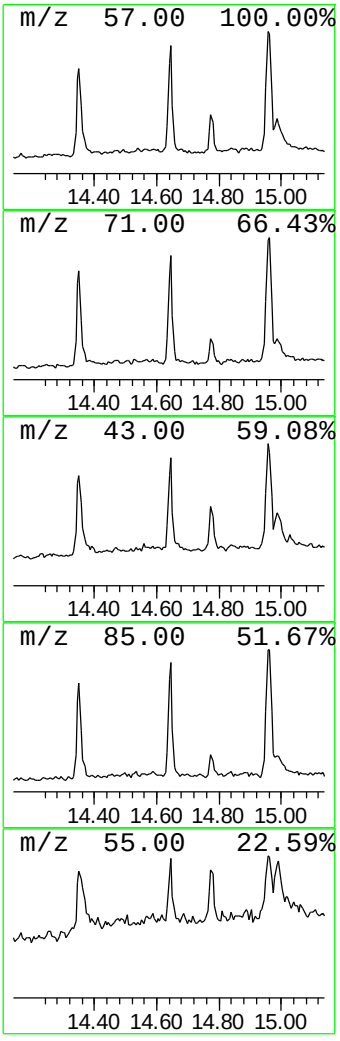
****

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.53 ng	220874	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	96
2	Heptacosane	380	C27H56	000593-49-7	94
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5	Tricosane	324	C23H48	000638-67-5	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

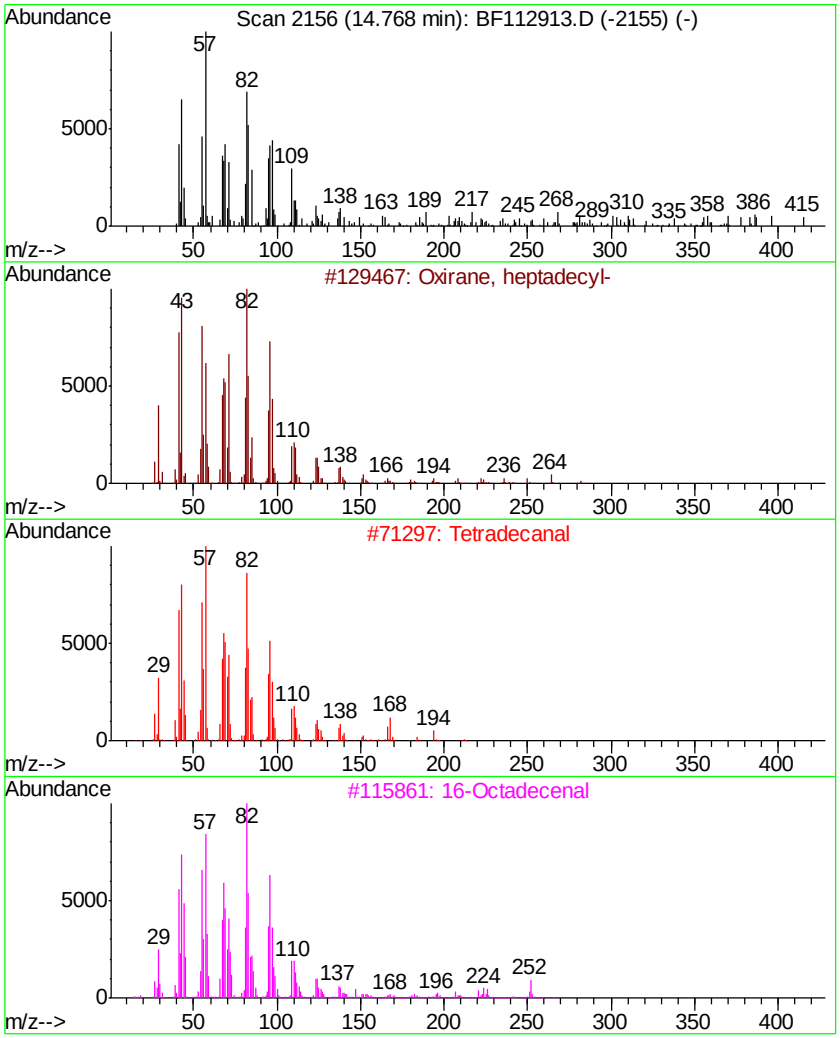
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

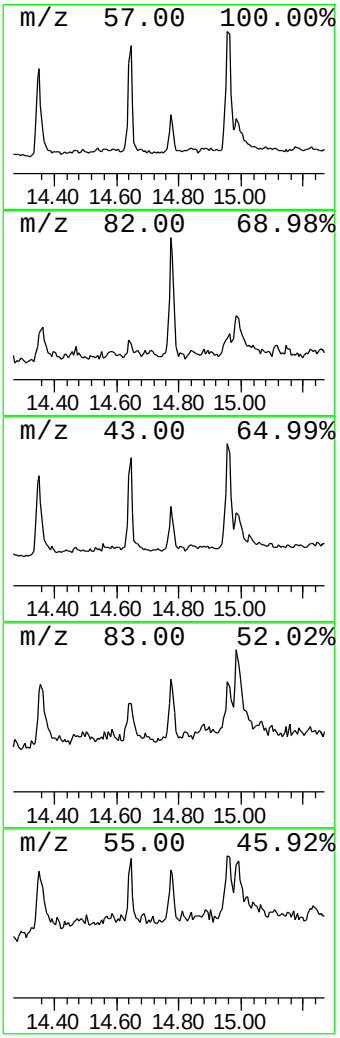
****

Peak Number 7 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.10 ng	150944	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
2	Tetradecanal	212	C14H28O	000124-25-4	90
3	16-Octadecenal	266	C18H34O	056554-87-1	89
4	Tetracosanal	352	C24H48O	057866-08-7	87
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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

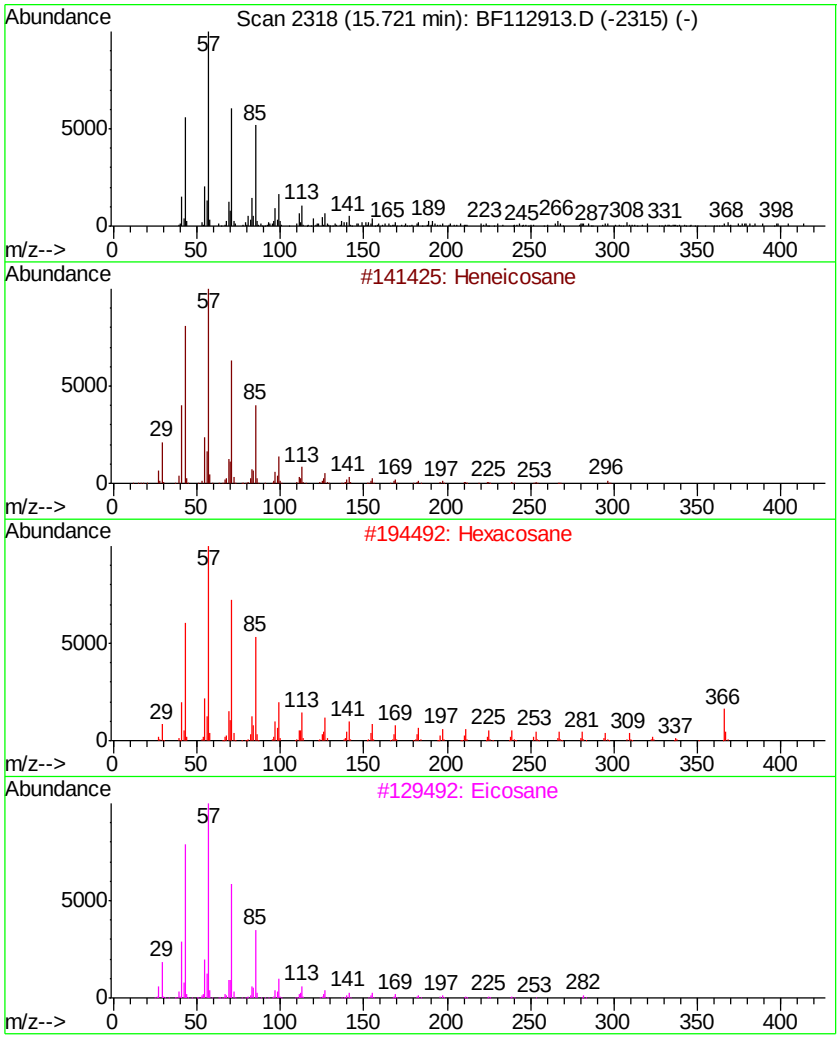
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

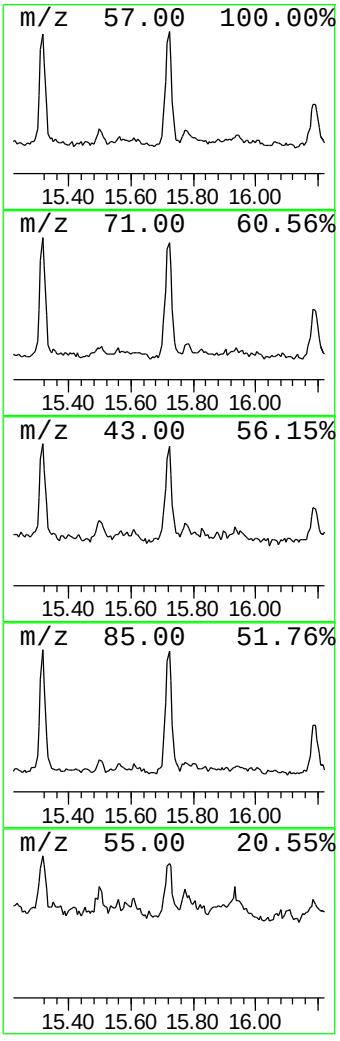
****

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.65 ng	226501	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Hexacosane	366	C26H54	000630-01-3	93
3	Eicosane	282	C20H42	000112-95-8	93
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030619\
Data File : BF112913.D
Acq On : 7 Mar 2019 6:11
Operator : JU/SJ
Sample : K1705-13 2X
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW024-022719

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	35.6	ng	1798050	1	6.73	1009940	20.0
n-Hexadecanoic acid	11.77	5.9	ng	384373	4	11.24	1308350	20.0
Cyclodocosane, et...	13.73	2.7	ng	233691	5	13.86	1733940	20.0
Eicosane	14.35	4.8	ng	415421	5	13.86	1733940	20.0
Tetracosane	14.64	4.5	ng	220874	6	15.27	974832	20.0
Oxirane, heptadecyl-	14.77	3.1	ng	150944	6	15.27	974832	20.0
Heneicosane	15.72	4.7	ng	226501	6	15.27	974832	20.0