LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112902.D
Acq On : 7 Mar 2019 1:10
Operator : JU/SJ
Sample : K1705-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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	5.345	549	554	557	rBV	4735775	5082681	91.49%	9.228%
2	6.369	723	728	746	rVB2	4490742	5555342	100.00%	10.086%
3	6.504	746	751	754	rBV	5244201	5200690	93.62%	9.443%
4	6.734	786	790	793	rBV	1472905	1304557	23.48%	2.369%
5	6.886	812	816	820	rBV	4290022	4116239	74.10%	7.474%
6	7.292	879	885	888	rBV	3335621	3314685	59.67%	6.018%
7	8.010	1003	1007	1027	rBV	1610314	1597977	28.76%	2.901%
8	9.086	1185	1190	1204	rBV	4976498	4984523	89.72%	9.050%
9	9.222	1210	1213	1222	rVB2	48047	71753	1.29%	0.130%
10	9.480	1253	1257	1263	rBV	336960	319200	5.75%	0.580%
11	9.763	1300	1305	1309	rBV	1550036	1536035	27.65%	2.789%
12	10.545	1433	1438	1449	rBV	3238321	3224144	58.04%	5.854%
13	11.239	1552	1556	1558	rBV	1441433	1472962	26.51%	2.674%
14	11.257	1558	1559	1563	rVV	389500	316336	5.69%	0.574%
15	11.310	1563	1568	1572	rVB	77856	94090	1.69%	0.171%
16	11.739	1638	1641	1643	rBV	78340	70188	1.26%	0.127%
17	11.774	1643	1647	1652	rVV2	633980	726975	13.09%	1.320%
18	11.845	1656	1659	1662	rBV	74694	77217	1.39%	0.140%
19	12.286	1731	1734	1737	rBV	64890	76187	1.37%	0.138%
20	12.363	1745	1747	1753	rVB2	48292	65936	1.19%	0.120%
21	12.439	1757	1760	1764	rBV	509065	482406	8.68%	0.876%
22	12.557	1777	1780	1790	rBV3	203409	286129	5.15%	0.520%
23	12.668	1793	1799	1805	rVV2	477767	550078	9.90%	0.999%
24	12.721	1805	1808	1813	rVB3	38088	64789	1.17%	0.118%
25	12.815	1820	1824	1828	rBV	4374675	4229631	76.14%	7.679%
26	12.892	1831	1837	1840	rBV3	47034	80228	1.44%	0.146%
27	12.992	1852	1854	1858	rVB2	67607	70998	1.28%	0.129%
28	13.098	1868	1872	1875	rBV	85241	76056	1.37%	0.138%
29	13.298	1903	1906	1914	rVB8	37628	59008	1.06%	0.107%
30	13.498	1937	1940	1945	rBV	66634	86757	1.56%	0.158%
31	13.604	1955	1958	1962	rBV2	51965	78607	1.41%	0.143%
32	13.721	1972	1978	1985	rBV2	458677	643945	11.59%	1.169%
33	13.857	1996	2001	2004	rBV3	3168111	3277806	59.00%	5.951%
34	13.880	2004	2005	2012	rVB	292437	272017	4.90%	0.494%

LSC Area Percent Report

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Sample : K1705-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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	14.045	2030	2033	2036	rBV2	77406	78461	1.41%	0.142%
36	14.245	2064	2067	2070	rVB	71333	63683	1.15%	0.116%
37	14.280	2070	2073	2076	rVB2	56954	62891	1.13%	0.114%
38	14.351	2081	2085	2097	rVB2	319843	572092	10.30%	1.039%
39	14.639	2131	2134	2141	rVV	135754	155262	2.79%	0.282%
40	14.709	2143	2146	2150	rVV3	101593	111041	2.00%	0.202%
41	14.774	2154	2157	2162	rVB2	102094	96543	1.74%	0.175%
42	14.862	2168	2172	2175	rBV	235334	332991	5.99%	0.605%
43	14.957	2184	2188	2190	rBV	246522	275739	4.96%	0.501%
44	14.986	2190	2193	2203	rVB2	241042	404286	7.28%	0.734%
45	15.145	2217	2220	2226	rVB	120160	143618	2.59%	0.261%
46	15.204	2226	2230	2235	rBV	181323	202436	3.64%	0.368%
47	15.262	2235	2240	2245	rBV	1378984	1715140	30.87%	3.114%
48	15.309	2245	2248	2253	rVB	167713	222251	4.00%	0.404%
49	15.715	2312	2317	2322	rBV	267447	380709	6.85%	0.691%
50	15.774	2322	2327	2334	rBV3	127241	308534	5.55%	0.560%
51	16.186	2392	2397	2401	rBV2	99959	169264	3.05%	0.307%
52	16.445	2437	2441	2448	rVB3	60069	116095	2.09%	0.211%
53	16.615	2466	2470	2476	rBV2	52438	87760	1.58%	0.159%
54	16.733	2485	2490	2494	rBV2	62345	112459	2.02%	0.204%

Sum of corrected areas: 55077427

LSC Report - Integrated Chromatogram

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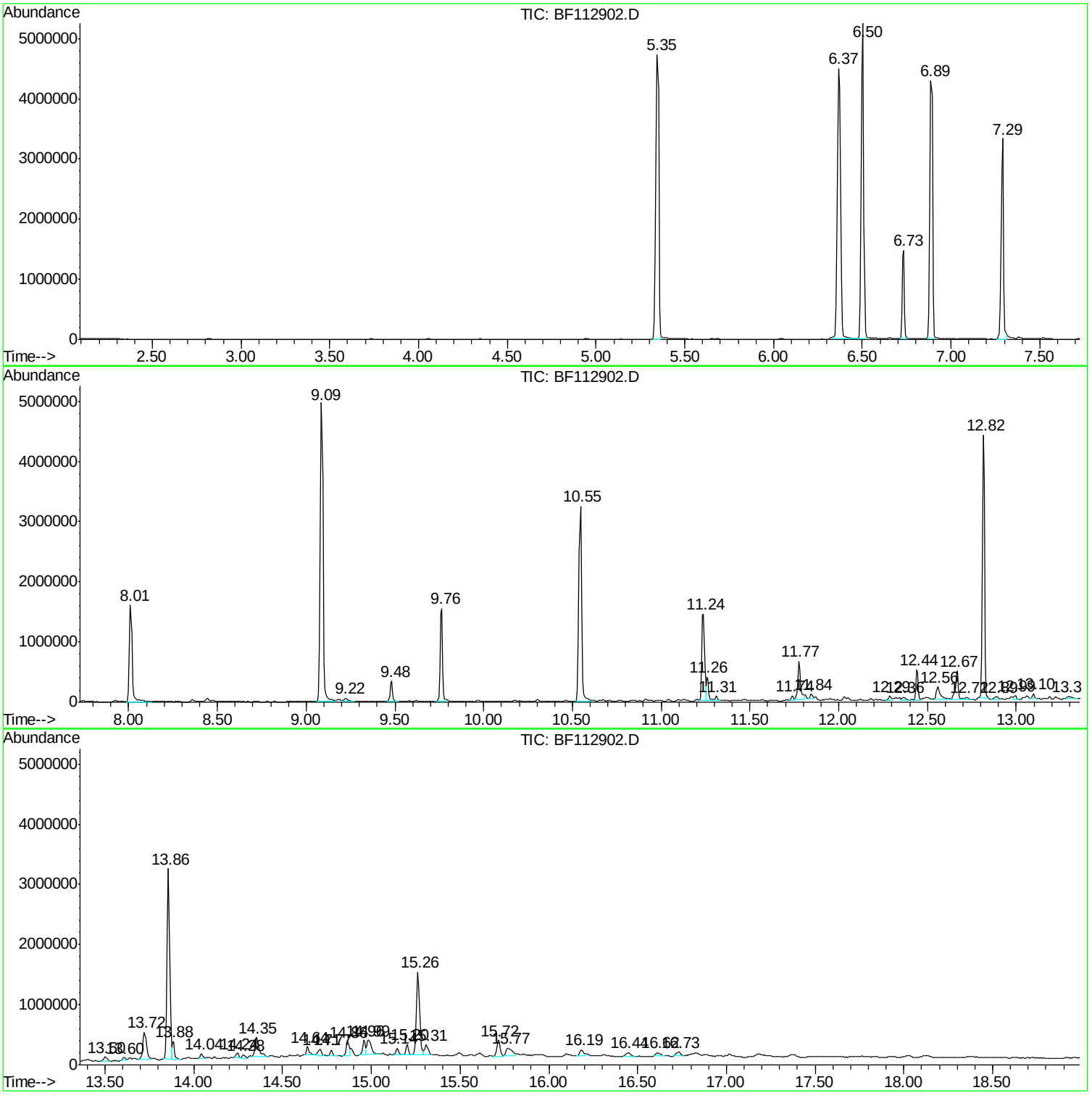
Sample : K1705-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-028-SW008-022719

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 : BF112902.D
Acq On : 7 Mar 2019 1:10
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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

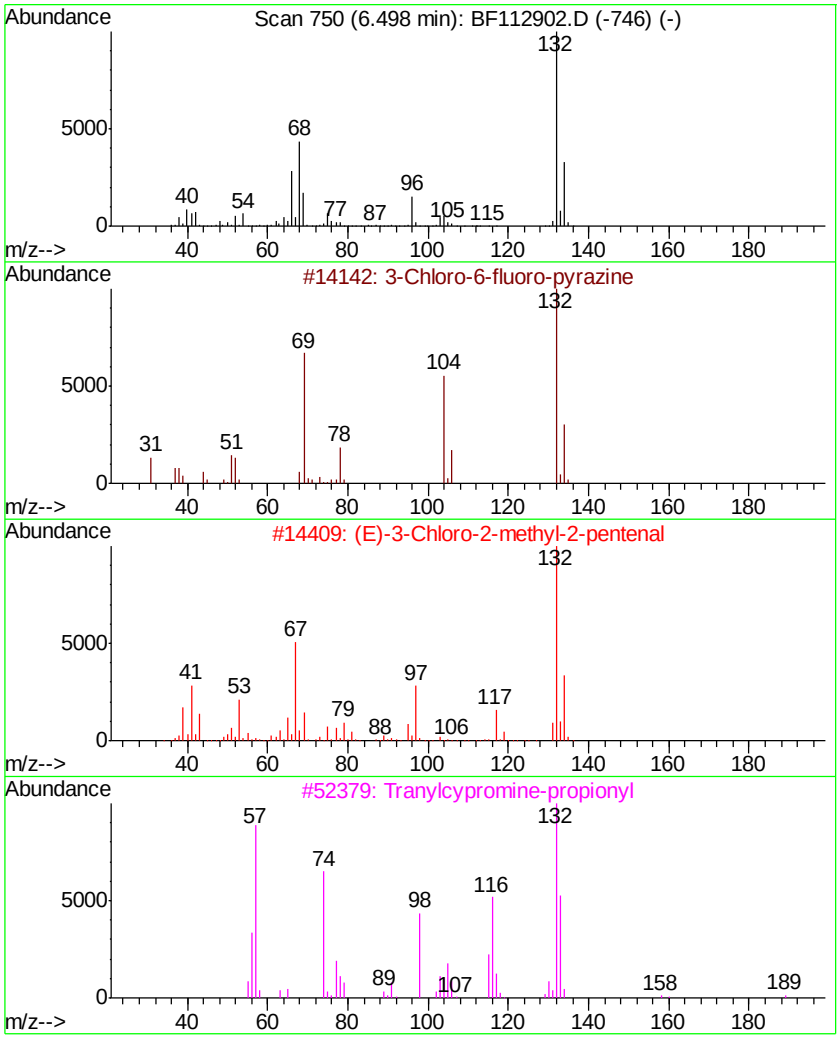
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

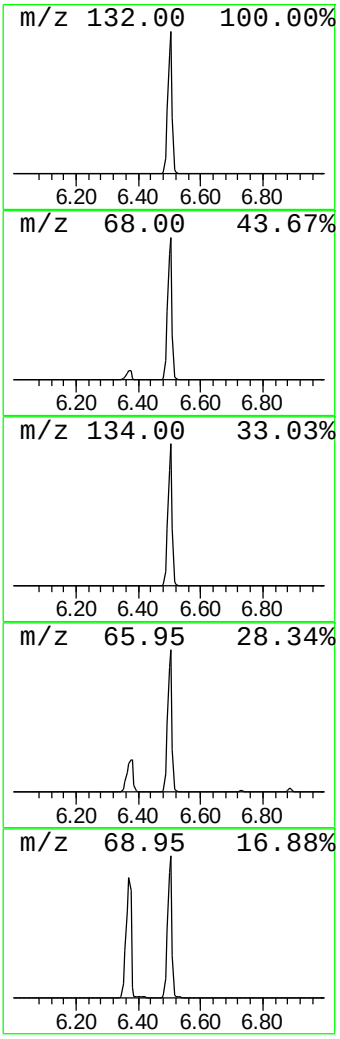
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	79.73 ng	5200690	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Data File : BF112902.D
Acq On : 7 Mar 2019 1:10
Operator : JU/SJ
Sample : K1705-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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

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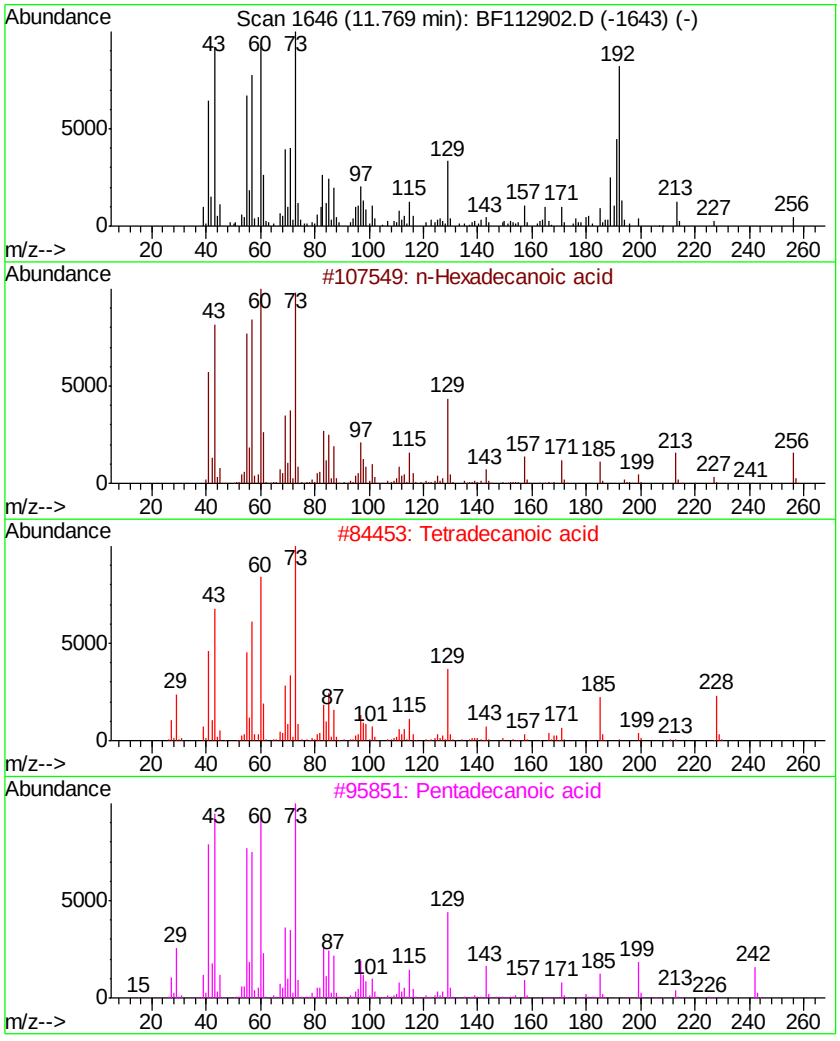
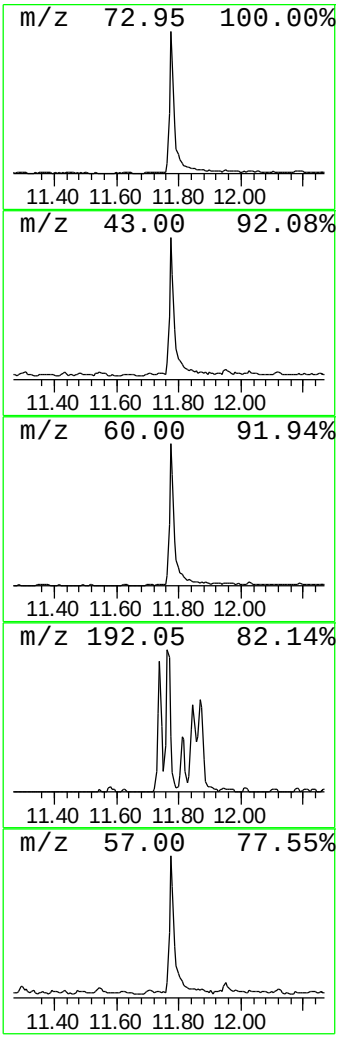
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	9.87 ng	726975	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	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Operator : JU/SJ
Sample : K1705-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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

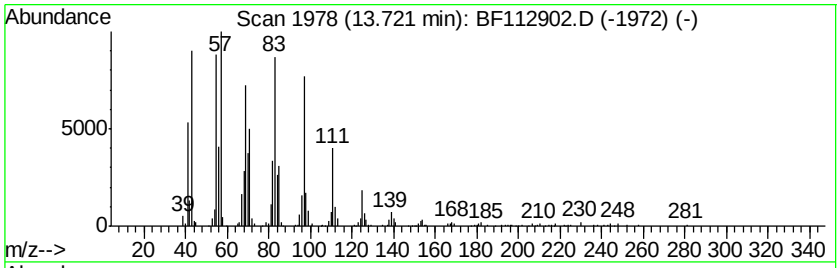
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

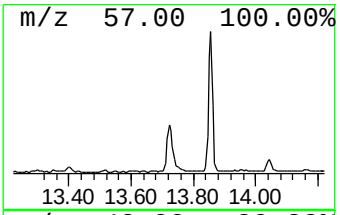
****

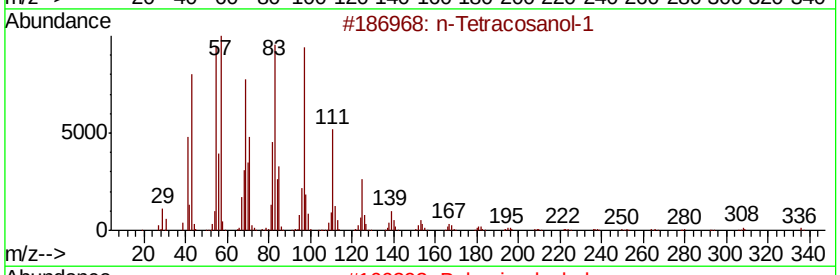
Peak Number 4 n-Tetracosanol-1 Concentration Rank 6

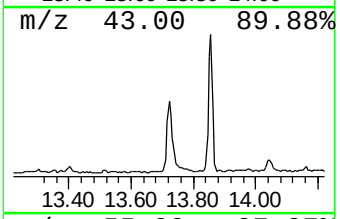
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.93 ng	643945	Chrysene-d12	13.86

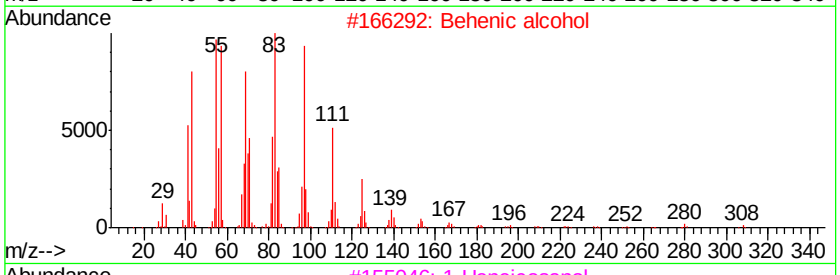
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	1-Docosene	308	C22H44	001599-67-3	91

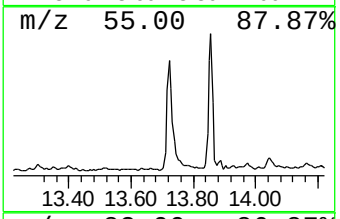


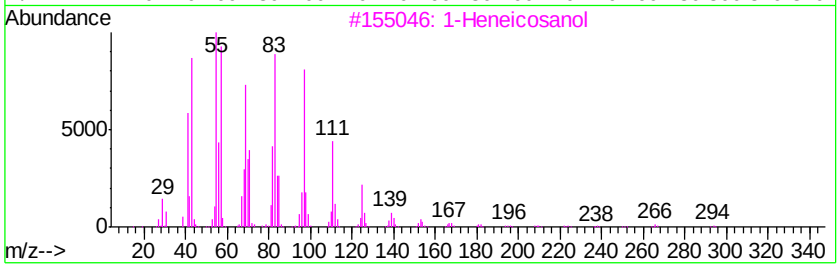


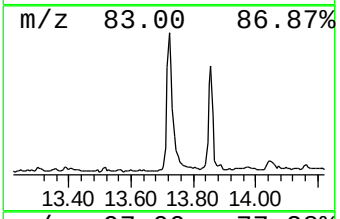


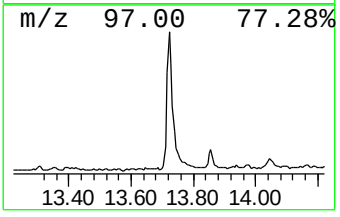












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ClientSampleId : EXT-028-SW008-022719

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

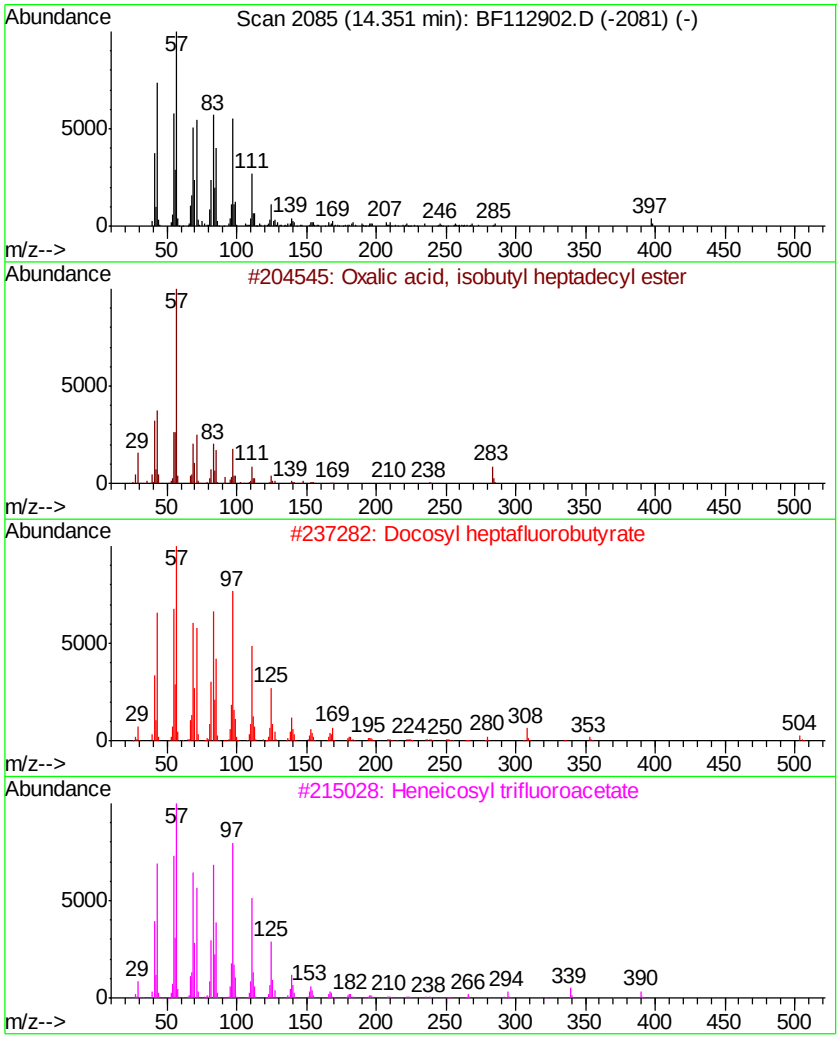
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

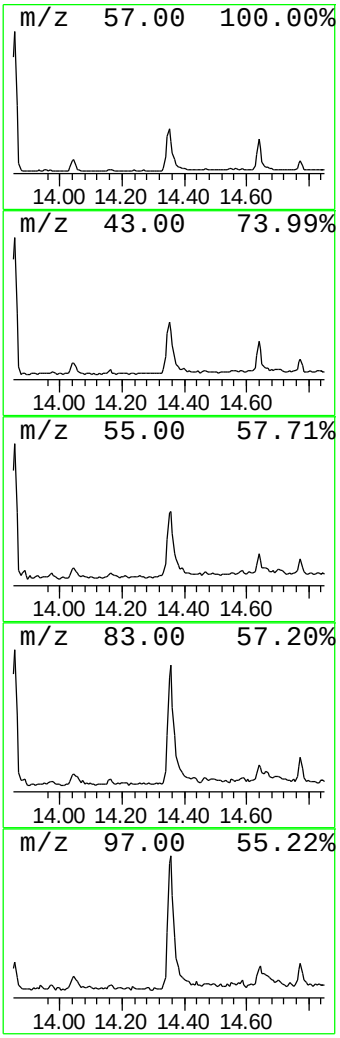
****

Peak Number 5 Oxalic acid, isobutyl hepta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.49 ng	572092	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
2	Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	91
3	Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	91
4	Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	83





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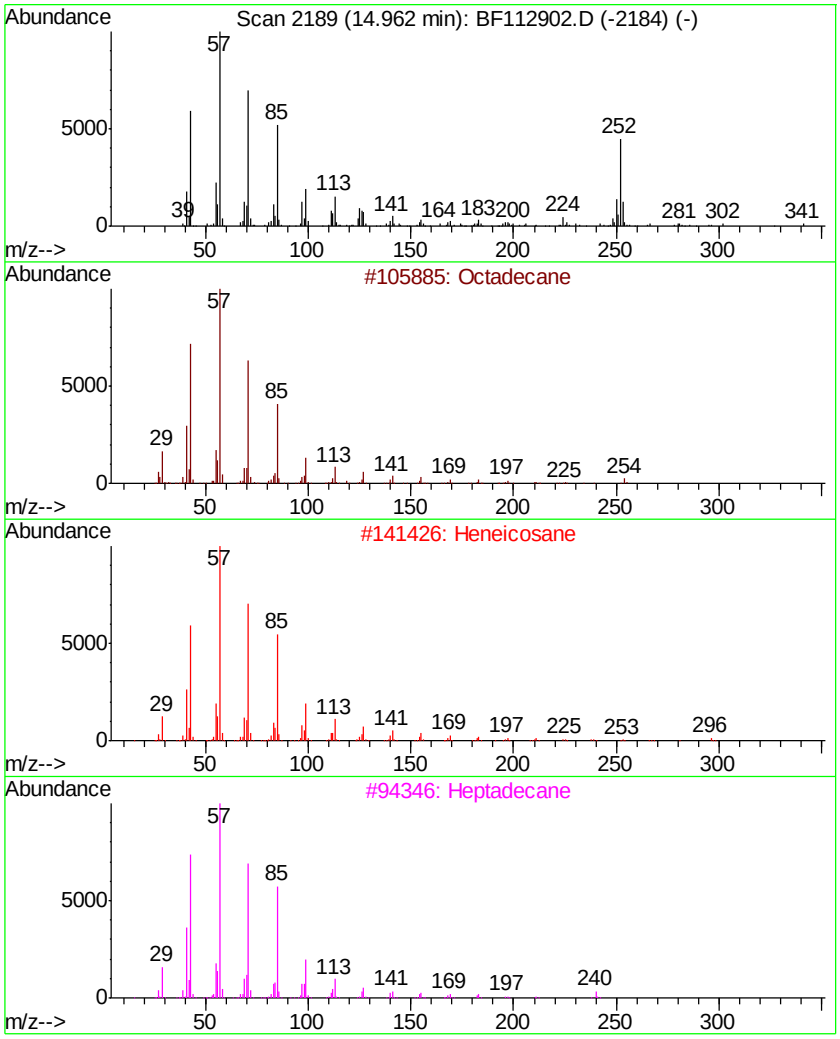
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

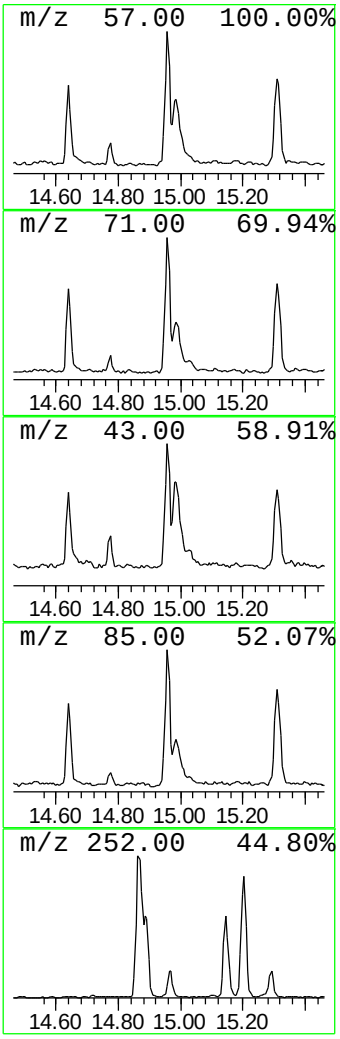
****

Peak Number 6 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.22 ng	275739	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Heneicosane	296	C21H44	000629-94-7	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
5	Pentacosane	352	C25H52	000629-99-2	80





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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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

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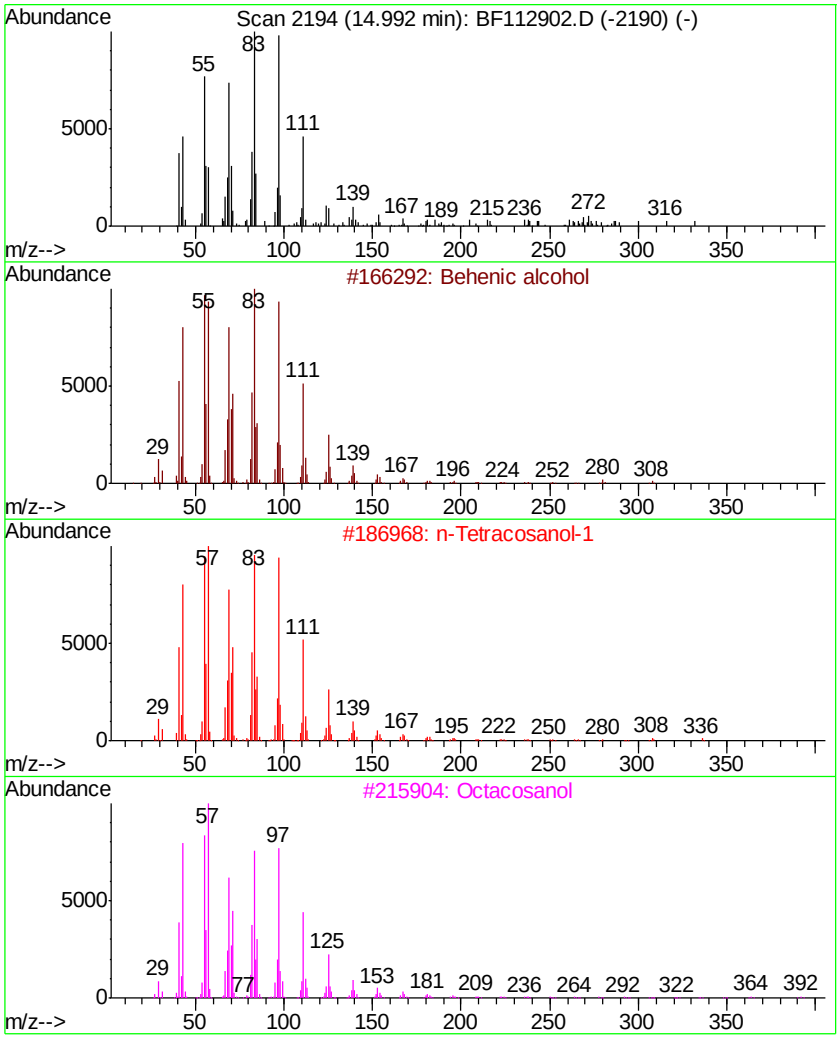
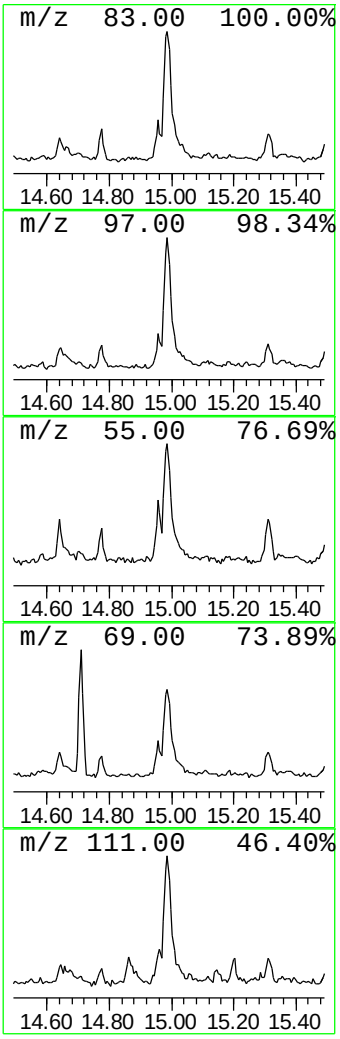
Peak Number 7 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	4.71 ng	404286	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	Octacosanol	410	C28H58O	000557-61-9	90
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	1-Eicosanol	298	C20H42O	000629-96-9	68





Library Search Compound Report

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Data File : BF112902.D
Acq On : 7 Mar 2019 1:10
Operator : JU/SJ
Sample : K1705-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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

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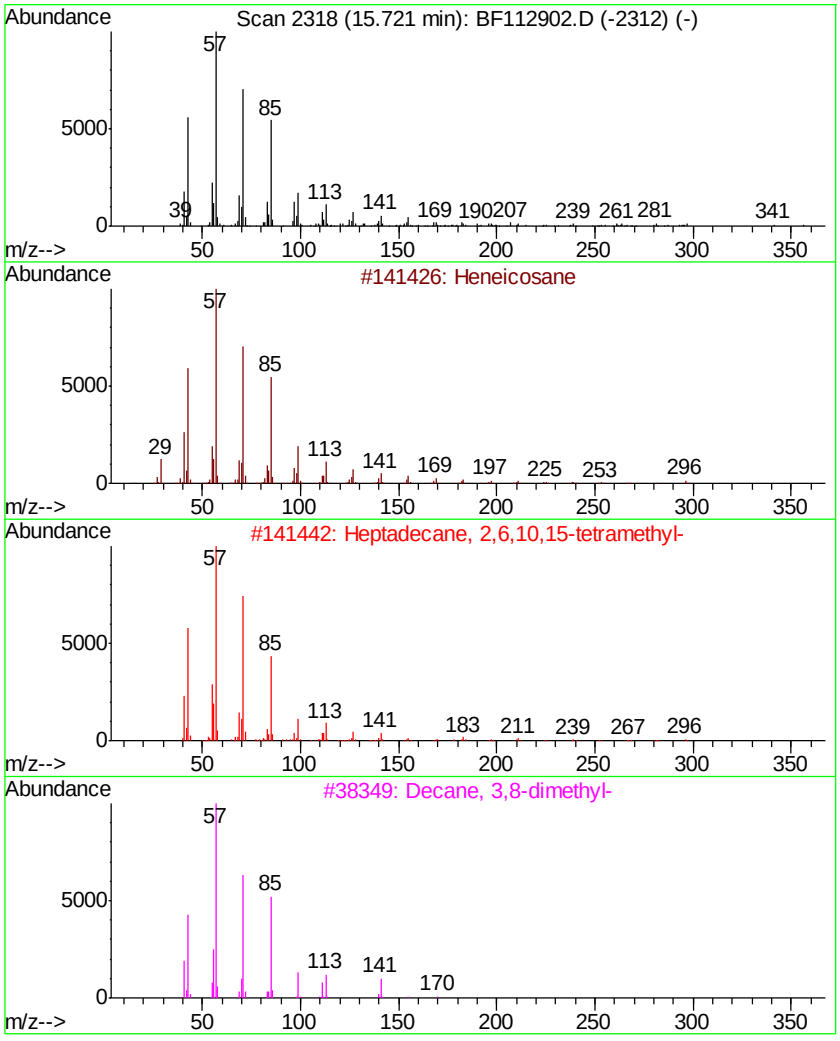
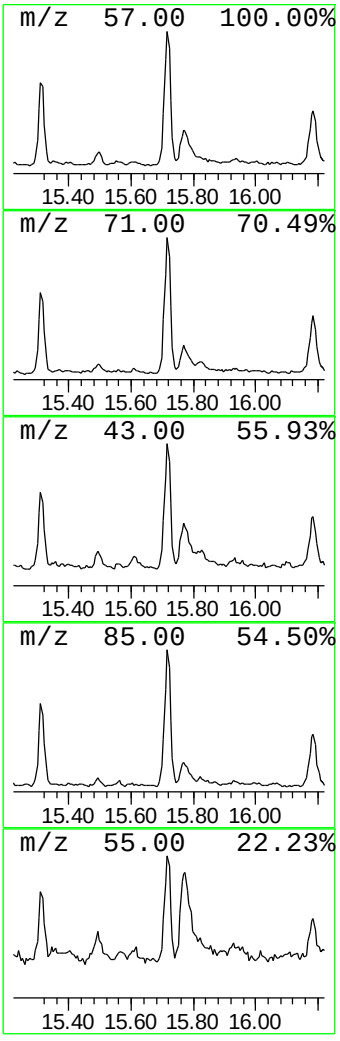
Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.44 ng	380709	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	86
5	Pentacosane	352	C25H52	000629-99-2	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030619\
Data File : BF112902.D
Acq On : 7 Mar 2019 1:10
Operator : JU/SJ
Sample : K1705-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW008-022719

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	79.7	ng	5200690	1	6.73	1304560	20.0
n-Hexadecanoic acid	11.77	9.9	ng	726975	4	11.24	1472960	20.0
n-Tetracosanol-1	13.72	3.9	ng	643945	5	13.86	3277810	20.0
Oxalic acid, isob...	14.35	3.5	ng	572092	5	13.86	3277810	20.0
Octadecane	14.96	3.2	ng	275739	6	15.26	1715140	20.0
Behenic alcohol	14.99	4.7	ng	404286	6	15.26	1715140	20.0
Heneicosane	15.72	4.4	ng	380709	6	15.26	1715140	20.0