LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
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	5.357	550	556	559	rBV	3885793	4030301	88.29%	9.223%
2	6.381	718	730	734	rBV	4016206	4564631	100.00%	10.446%
3	6.510	747	752	755	rBV	4319204	4323811	94.72%	9.895%
4	6.739	787	791	794	rBV	1275419	1004175	22.00%	2.298%
5	6.898	813	818	821	rBV	3855032	3331433	72.98%	7.624%
6	7.298	881	886	889	rBV	2700214	2655123	58.17%	6.076%
7	8.022	1005	1009	1029	rBV	1271705	1253076	27.45%	2.868%
8	8.369	1064	1068	1075	rBV	31105	52611	1.15%	0.120%
9	8.451	1079	1082	1086	rBV	89238	88514	1.94%	0.203%
10	9.098	1187	1192	1195	rBV	4542022	4041457	88.54%	9.249%
11	9.233	1212	1215	1224	rVB	38159	62209	1.36%	0.142%
12	9.486	1255	1258	1265	rBV	284052	264555	5.80%	0.605%
13	9.769	1302	1306	1311	rBV2	1294025	1237089	27.10%	2.831%
14	10.557	1435	1440	1453	rBV	2852657	2791292	61.15%	6.388%
15	11.251	1554	1558	1560	rBV	1227977	1181304	25.88%	2.703%
16	11.269	1560	1561	1565	rVV	297011	251885	5.52%	0.576%
17	11.322	1568	1570	1575	rVB	60039	55643	1.22%	0.127%
18	11.751	1640	1643	1645	rBV	65406	56450	1.24%	0.129%
19	11.786	1645	1649	1659	rVV3	540755	668634	14.65%	1.530%
20	11.857	1659	1661	1664	rBV	58159	61237	1.34%	0.140%
21	12.298	1733	1736	1739	rBV2	63238	66159	1.45%	0.151%
22	12.457	1759	1763	1766	rBV	435009	386355	8.46%	0.884%
23	12.569	1779	1782	1793	rVV3	167112	236368	5.18%	0.541%
24	12.680	1795	1801	1805	rVV2	374057	435129	9.53%	0.996%
25	12.833	1822	1827	1830	rBV	3847913	3648923	79.94%	8.350%
26	12.904	1834	1839	1843	rBV3	41318	63769	1.40%	0.146%
27	13.010	1855	1857	1860	rVB	65761	58673	1.29%	0.134%
28	13.051	1860	1864	1866	rBV4	39120	51467	1.13%	0.118%
29	13.116	1871	1875	1878	rBV	62041	69761	1.53%	0.160%
30	13.316	1905	1909	1916	rVB9	32228	56688	1.24%	0.130%
31	13.515	1940	1943	1948	rVB	65643	82687	1.81%	0.189%
32	13.621	1957	1961	1965	rBV2	51504	85968	1.88%	0.197%
33	13.733	1975	1980	1986	rBV2	456175	561287	12.30%	1.284%
34	13.874	1999	2004	2007	rBV2	2474786	2674702	58.60%	6.121%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
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

35	13.898	2007	2008	2015	rVB	246514	188656	4.13%	0.432%
36	14.057	2032	2035	2039	rVB2	77221	73271	1.61%	0.168%
37	14.363	2084	2087	2094	rBV2	317551	403713	8.84%	0.924%
38	14.657	2134	2137	2144	rVB2	99666	136023	2.98%	0.311%
39	14.727	2146	2149	2153	rVV2	80835	84313	1.85%	0.193%
40	14.792	2157	2160	2166	rVB3	80451	75339	1.65%	0.172%
41	14.886	2172	2176	2179	rBV	134125	209582	4.59%	0.480%
42	14.980	2188	2192	2193	rBV	141345	167559	3.67%	0.383%
43	14.998	2193	2195	2201	rVB	236964	284630	6.24%	0.651%
44	15.168	2221	2224	2230	rVB	63979	79715	1.75%	0.182%
45	15.221	2230	2233	2238	rVB	85602	102379	2.24%	0.234%
46	15.286	2239	2244	2249	rBV	793265	927367	20.32%	2.122%
47	15.333	2249	2252	2256	rVB	97925	110863	2.43%	0.254%
48	15.739	2317	2321	2325	rBV	140699	194871	4.27%	0.446%
49	15.786	2325	2329	2338	rVV3	105779	206635	4.53%	0.473%

Sum of corrected areas: 43698282

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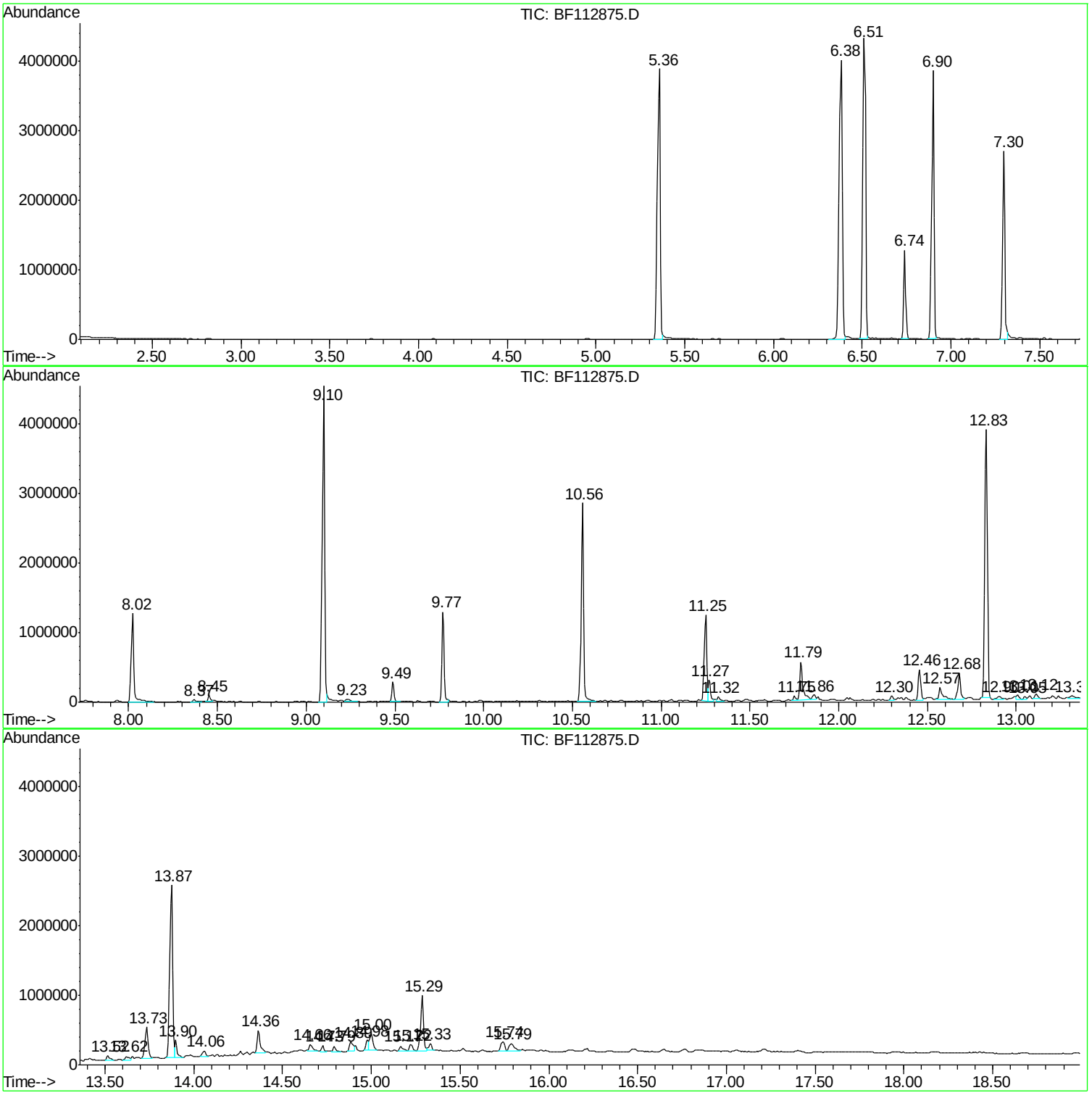
Instrument :
BNA_F
ClientSampleId :
EXT-028-SW008-022719

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
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

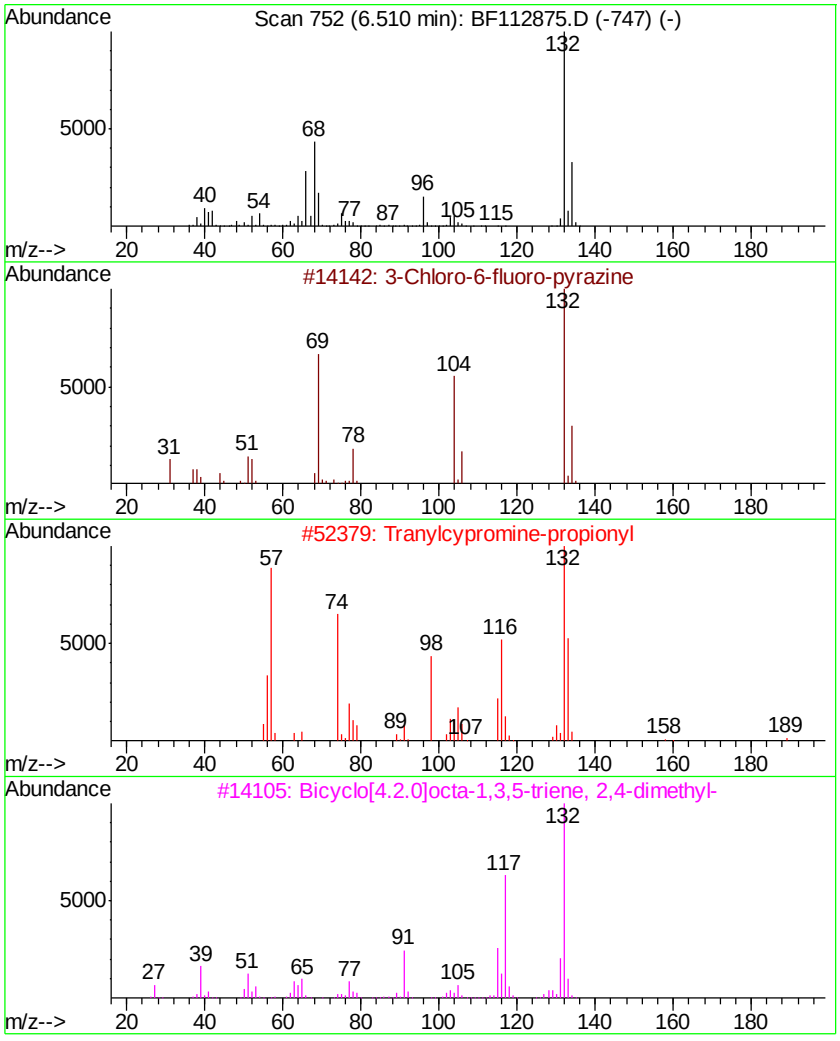
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

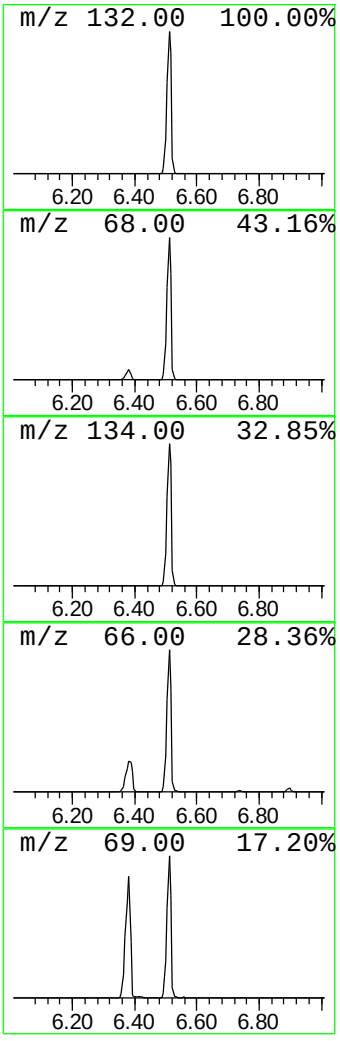
****

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	86.12 ng	4323810	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
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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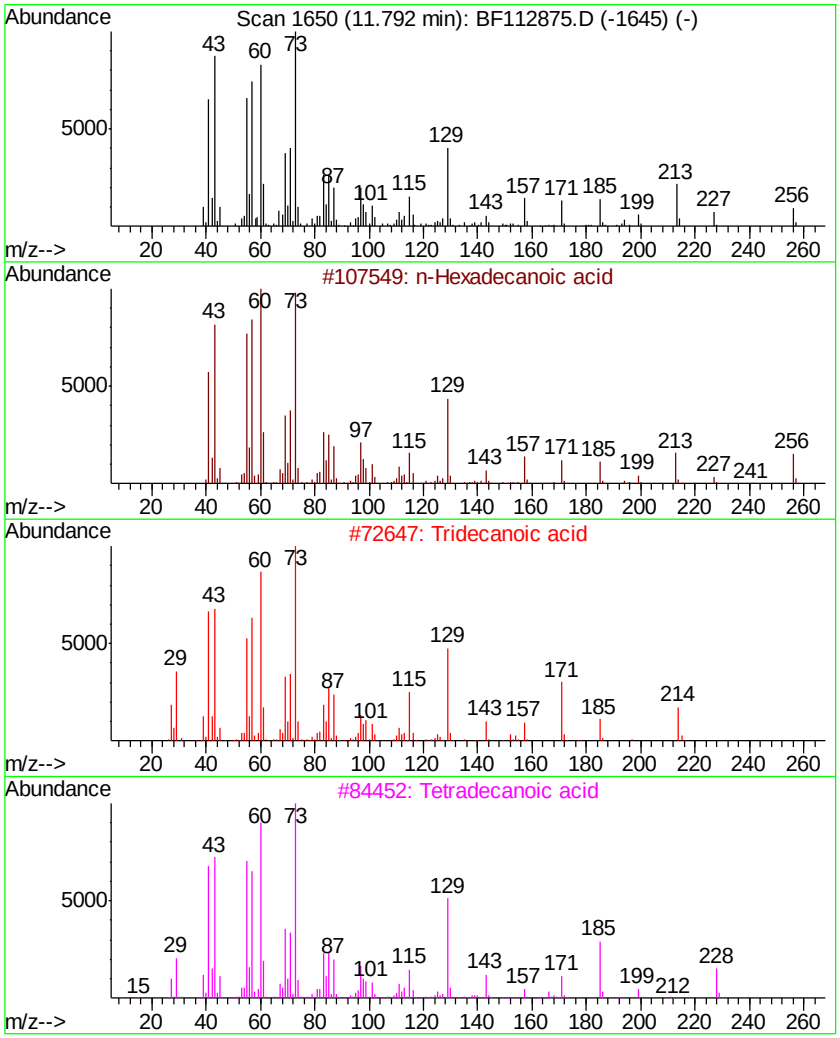
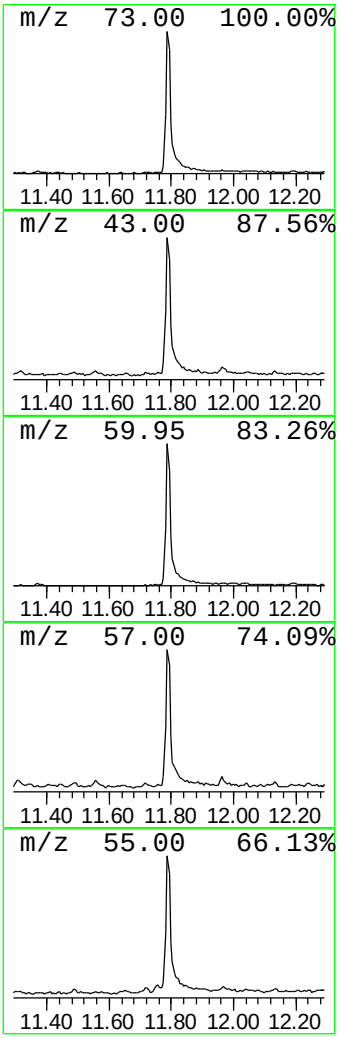
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	11.32 ng	668634	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
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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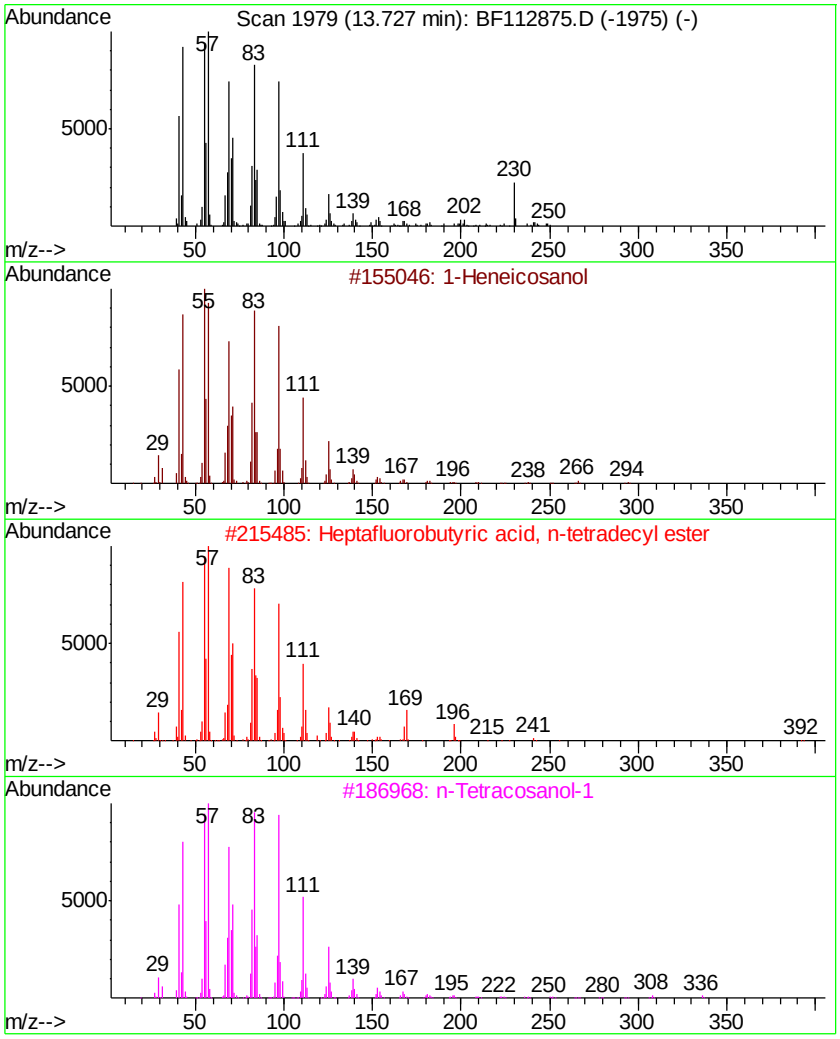
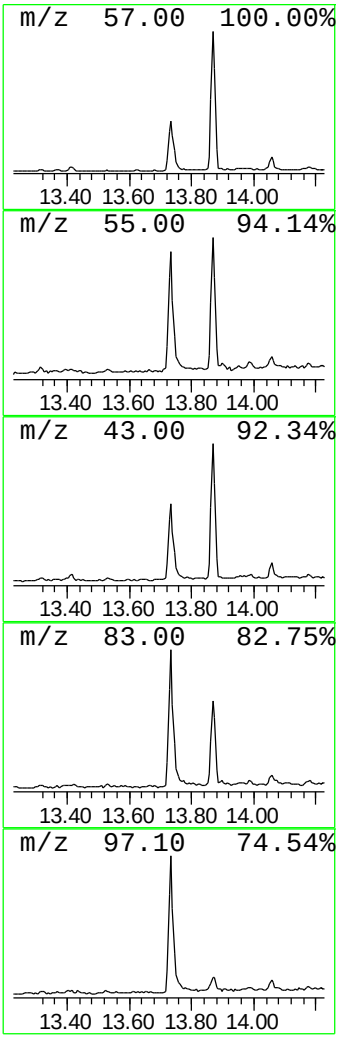
Peak Number 4 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.20 ng	561287	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
Operator : JU/SJ
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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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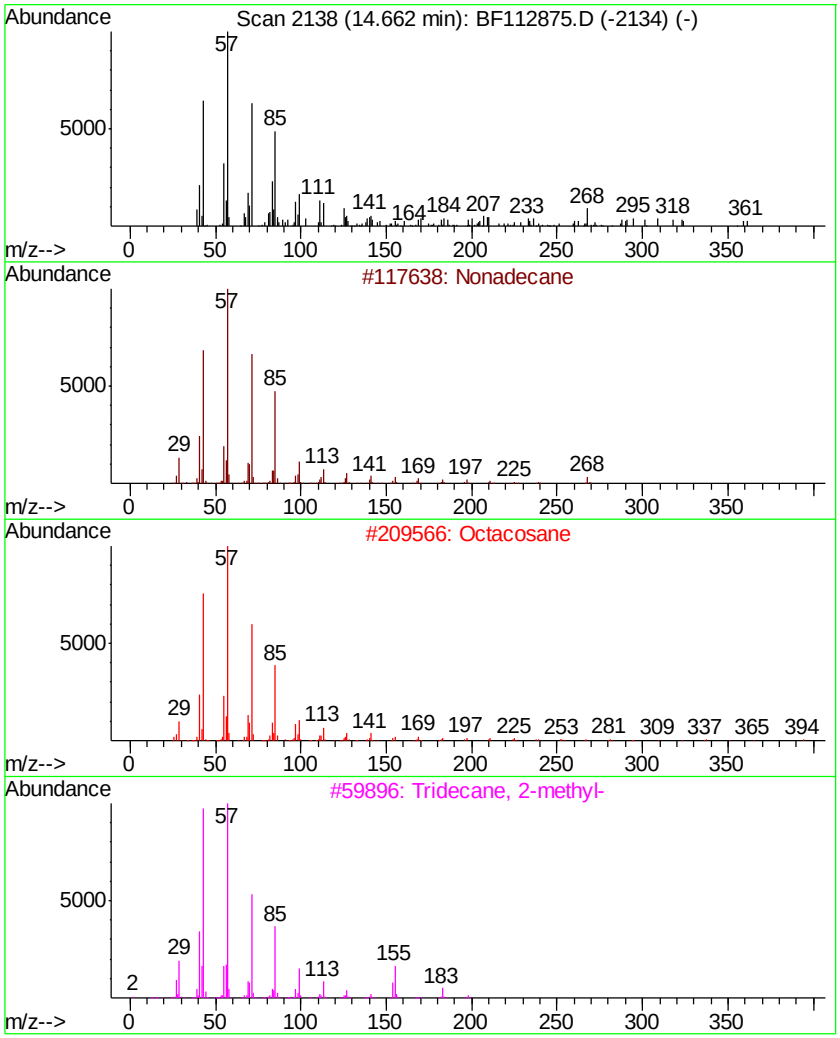
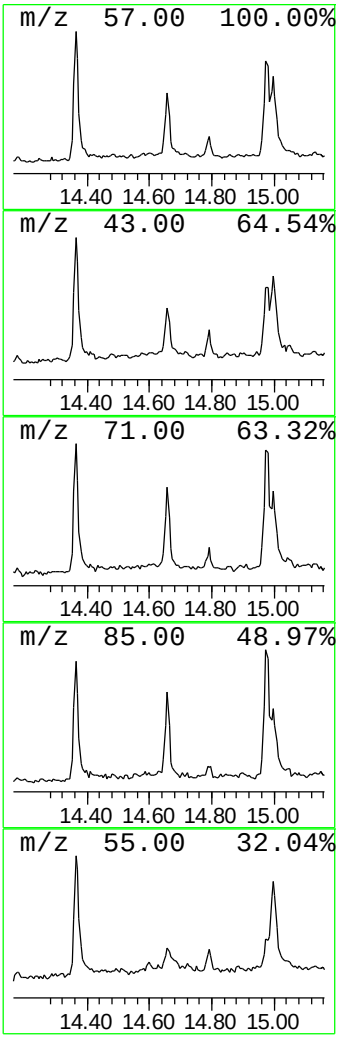
Peak Number 6 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.93 ng	136023	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	80
2	Octacosane	394	C28H58	000630-02-4	74
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	74
4	Hexadecane	226	C16H34	000544-76-3	74
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72





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Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
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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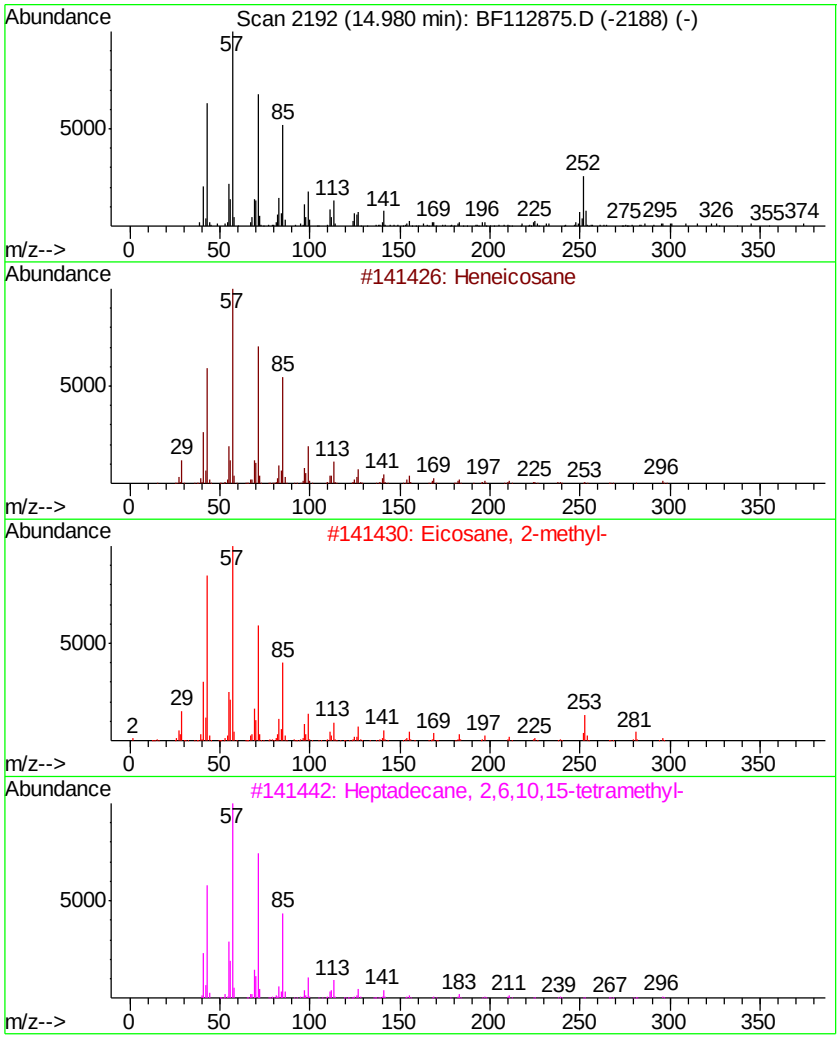
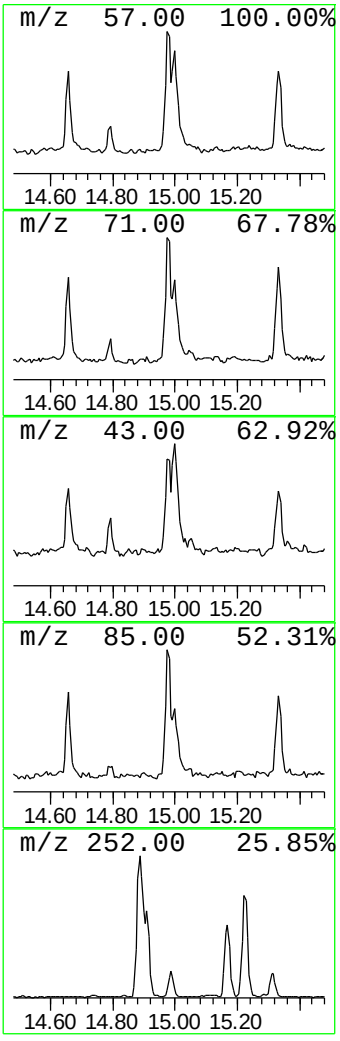
Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.61 ng	167559	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89
4	Octacosane	394	C28H58	000630-02-4	81
5	Pentacosane	352	C25H52	000629-99-2	81





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Acq On : 6 Mar 2019 2:00
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

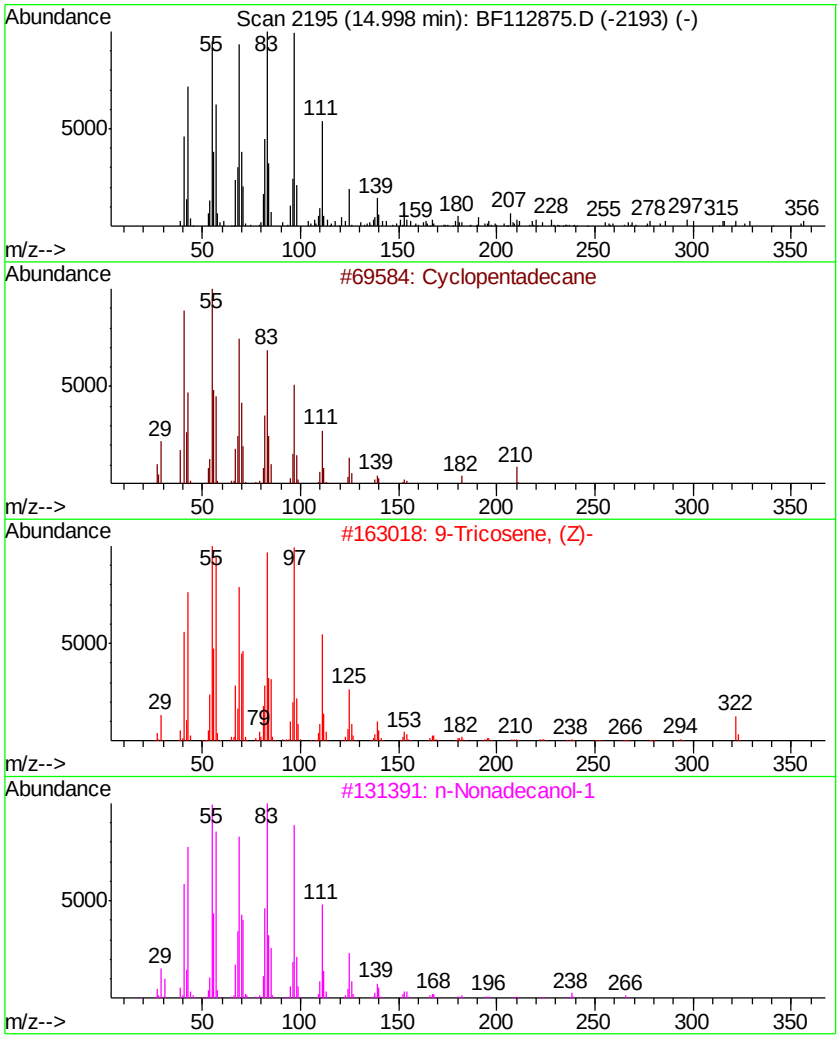
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

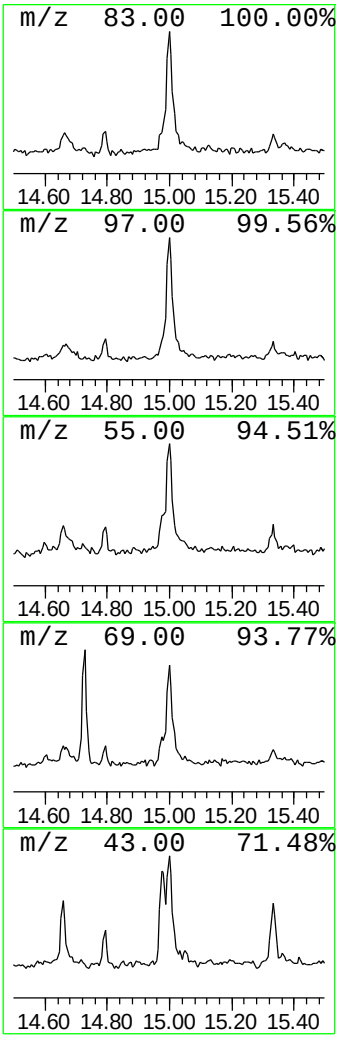
****

Peak Number 8 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	6.14 ng	284630	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





Library Search Compound Report

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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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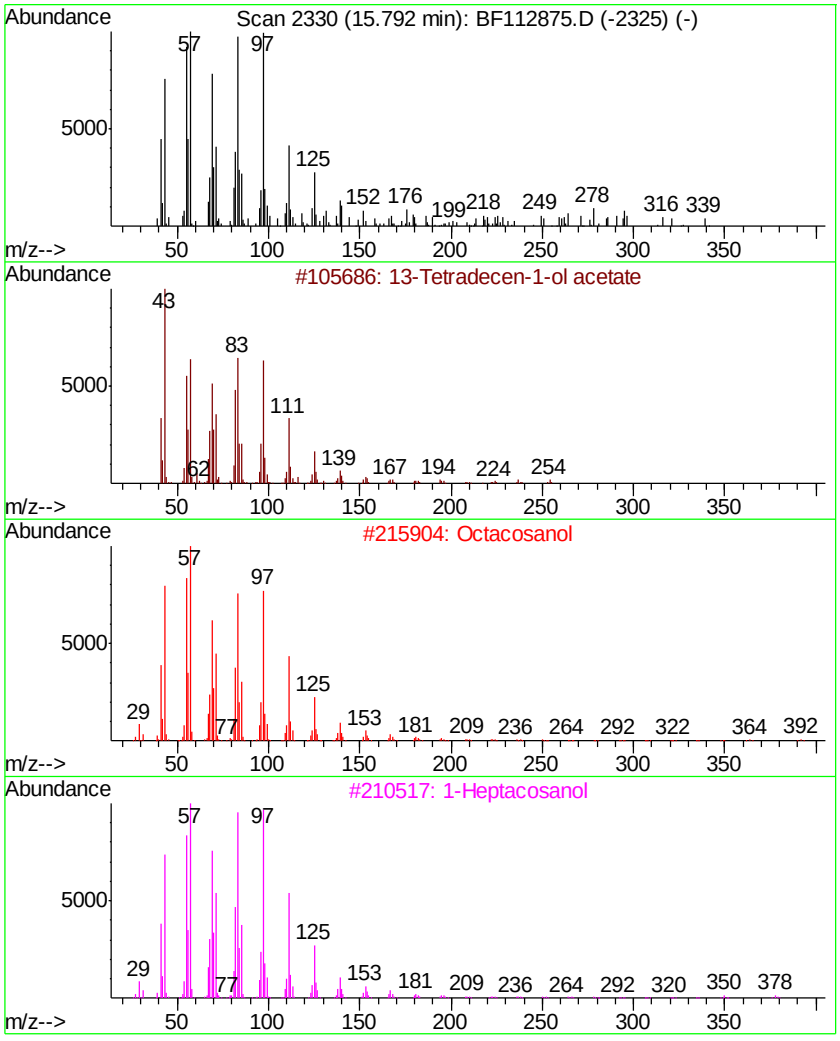
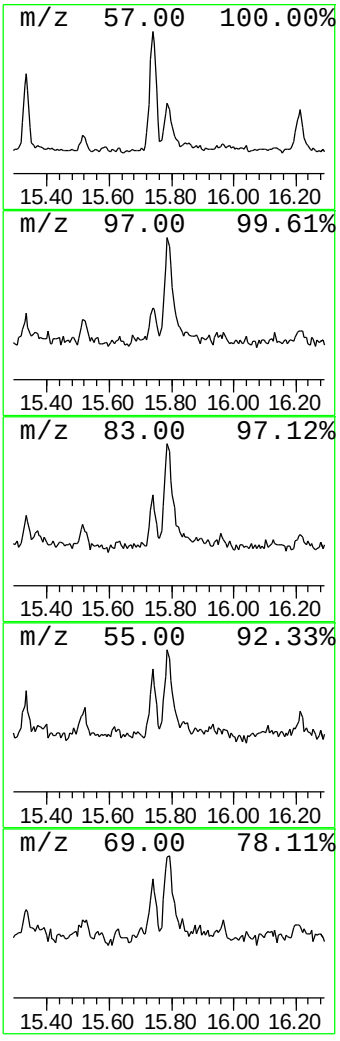
Peak Number 10 13-Tetradecen-1-ol acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	4.46 ng	206635	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
2	Octacosanol	410	C28H58O	000557-61-9	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	90
4	Cyclotetracosane	336	C24H48	000297-03-0	76
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
Data File : BF112875.D
Acq On : 6 Mar 2019 2:00
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
unknown6.51	6.51	86.1	ng	4323810	1	6.74	1004180	20.0
n-Hexadecanoic acid	11.79	11.3	ng	668634	4	11.25	1181300	20.0
1-Heneicosanol	13.73	4.2	ng	561287	5	13.87	2674700	20.0
Nonadecane	14.66	2.9	ng	136023	6	15.29	927367	20.0
Heneicosane	14.98	3.6	ng	167559	6	15.29	927367	20.0
Cyclopentadecane	15.00	6.1	ng	284630	6	15.29	927367	20.0
13-Tetradecen-1-o...	15.79	4.5	ng	206635	6	15.29	927367	20.0