LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109396.D
Acq On : 27 Sep 2018 19:16
Operator : JU/SJ
Sample : J5077-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

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-BF092218.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	4.893	474	477	486	rBV	47538	57624	3.38%	0.310%
2	5.316	544	549	552	rBV	1594365	1456122	85.32%	7.831%
3	6.346	719	724	734	rBV	1575122	1554825	91.10%	8.362%
4	6.475	742	746	749	rBV	1880955	1561285	91.48%	8.397%
5	6.704	782	785	789	rBV	765366	600711	35.20%	3.231%
6	6.863	808	812	815	rBV	1526300	1232212	72.20%	6.627%
7	7.263	876	880	883	rBV	1160341	966868	56.65%	5.200%
8	7.987	999	1003	1006	rBV	942858	756564	44.33%	4.069%
9	9.063	1182	1186	1189	rBV	2085342	1706670	100.00%	9.178%
10	9.457	1249	1253	1265	rVB	600088	504838	29.58%	2.715%
11	9.734	1296	1300	1304	rBV2	937480	829962	48.63%	4.464%
12	10.516	1430	1433	1444	rBV	1015491	917308	53.75%	4.933%
13	11.210	1548	1551	1554	rBV	901579	756765	44.34%	4.070%
14	11.233	1554	1555	1558	rVB	78099	42416	2.49%	0.228%
15	11.751	1639	1643	1647	rBV2	94146	92276	5.41%	0.496%
16	12.416	1752	1756	1760	rVB	173905	155114	9.09%	0.834%
17	12.533	1771	1776	1780	rBV4	25111	32369	1.90%	0.174%
18	12.645	1789	1795	1798	rBV	156081	153785	9.01%	0.827%
19	12.792	1816	1820	1823	rVB	1539787	1258233	73.72%	6.767%
20	12.974	1848	1851	1854	rVB	21693	21617	1.27%	0.116%
21	13.039	1858	1862	1865	rBV	29973	32232	1.89%	0.173%
22	13.269	1899	1901	1906	rVB2	17908	20611	1.21%	0.111%
23	13.586	1952	1955	1958	rBV2	19529	20783	1.22%	0.112%
24	13.710	1973	1976	1990	rVB2	110276	200021	11.72%	1.076%
25	13.839	1993	1998	2000	rVV	803448	828333	48.54%	4.455%
26	13.863	2000	2002	2005	rVB	93699	71805	4.21%	0.386%
27	13.945	2013	2016	2019	rBV2	23377	28609	1.68%	0.154%
28	13.974	2019	2021	2024	rBV2	24189	21294	1.25%	0.115%
29	14.016	2025	2028	2031	rBV3	54326	60894	3.57%	0.327%
30	14.321	2077	2080	2082	rBV2	62194	59440	3.48%	0.320%
31	14.351	2082	2085	2092	rVB7	33571	69243	4.06%	0.372%
32	14.616	2127	2130	2134	rBV	63999	67971	3.98%	0.366%
33	14.686	2139	2142	2147	rVV	190921	180517	10.58%	0.971%
34	14.751	2150	2153	2157	rVB	97481	96913	5.68%	0.521%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J5077-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.845	2165	2169	2172	rBV	111889	170318	9.98%	0.916%
36	14.933	2180	2184	2187	rBV2	106778	124613	7.30%	0.670%
37	14.974	2187	2191	2198	rVV4	34099	75091	4.40%	0.404%
38	15.121	2213	2216	2222	rVB	70865	95304	5.58%	0.513%
39	15.174	2222	2225	2231	rVB	78869	97360	5.70%	0.524%
40	15.239	2231	2236	2240	rBV	615896	717254	42.03%	3.857%
41	15.286	2240	2244	2248	rVB2	89388	120417	7.06%	0.648%
42	15.463	2271	2274	2278	rVB3	28488	36040	2.11%	0.194%
43	15.686	2307	2312	2318	rVB	133113	183421	10.75%	0.986%
44	15.757	2321	2324	2329	rBV6	20327	36373	2.13%	0.196%
45	16.145	2386	2390	2394	rBV	57874	89039	5.22%	0.479%
46	16.410	2431	2435	2444	rVB8	25935	51774	3.03%	0.278%
47	16.580	2460	2464	2472	rVB2	34550	62888	3.68%	0.338%
48	16.686	2478	2482	2489	rVB	48890	88424	5.18%	0.476%
49	16.980	2529	2532	2543	rVB	32462	67428	3.95%	0.363%
50	17.315	2586	2589	2600	rVB9	28696	70549	4.13%	0.379%
51	17.968	2695	2700	2708	rVB10	35440	91693	5.37%	0.493%

Sum of corrected areas: 18594216

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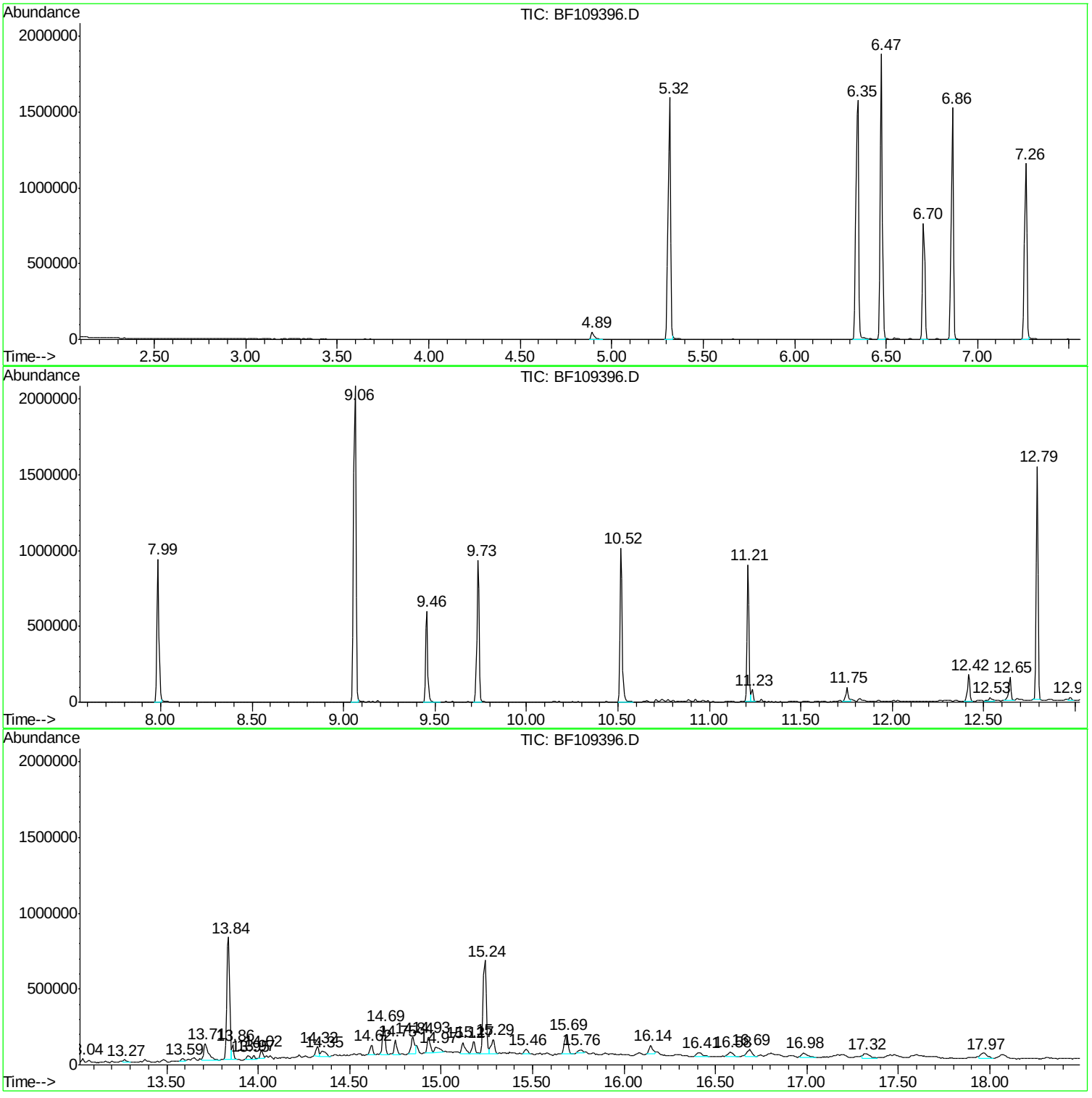
Instrument :
BNA_F
ClientSampleId :
PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

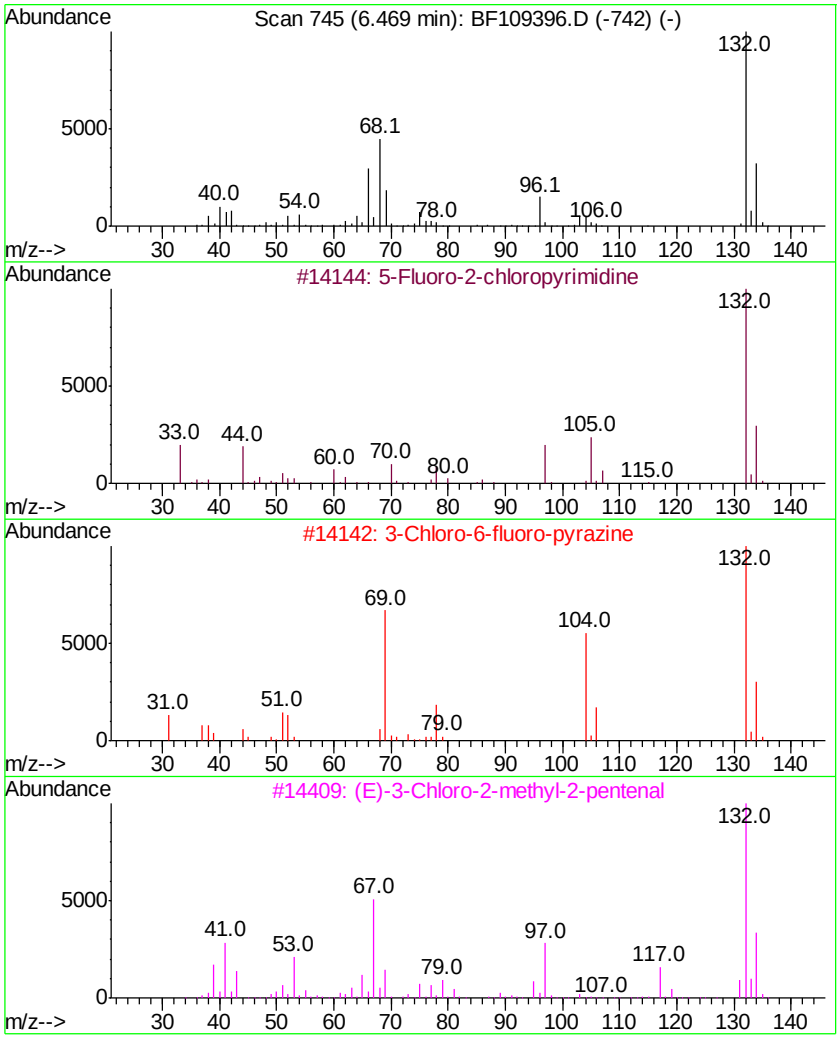
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

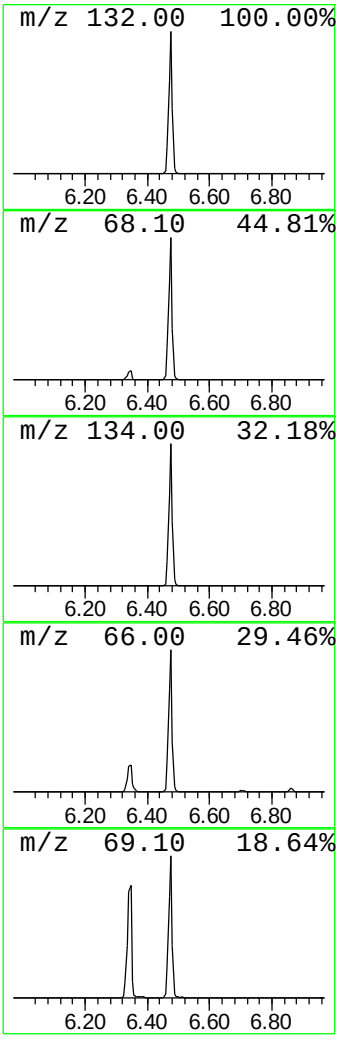
****

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	51.98 ng	1561290	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Misc :
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Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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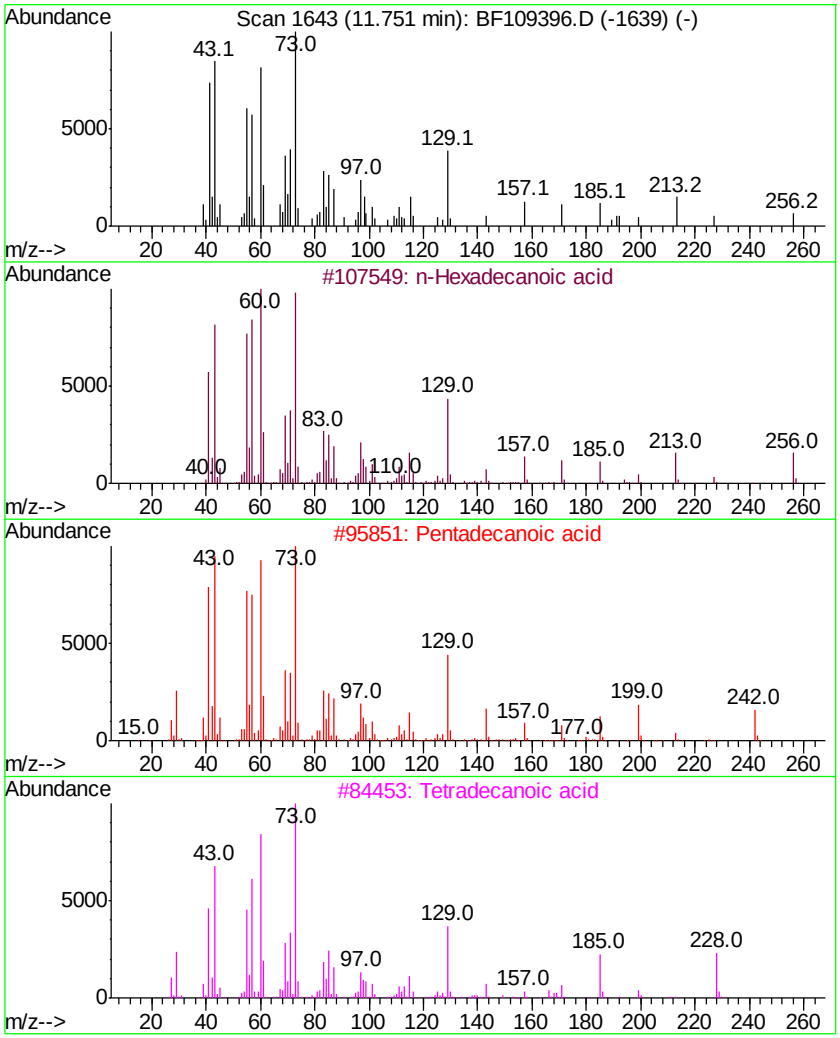
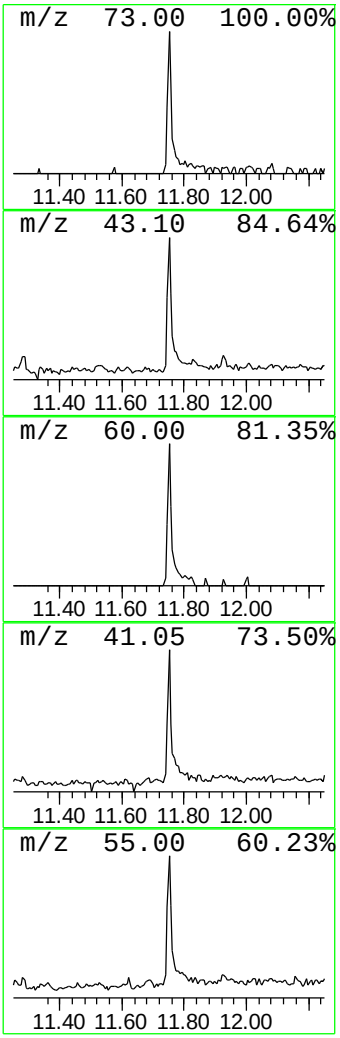
Peak Number 3 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.44 ng	92276	Phenanthrene-d10	11.21

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
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Sample : J5077-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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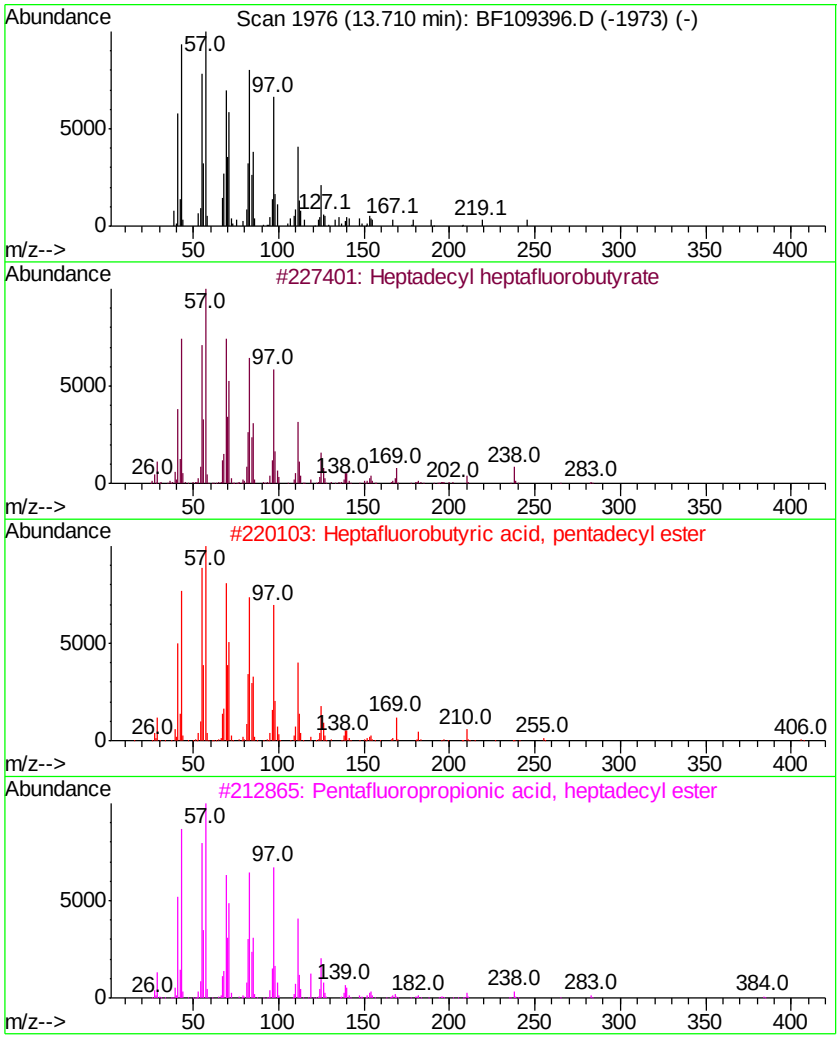
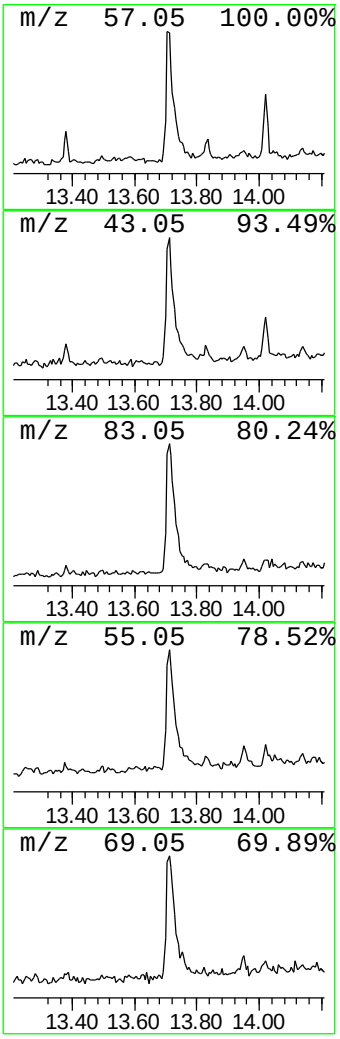
Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	4.83 ng	200021	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





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Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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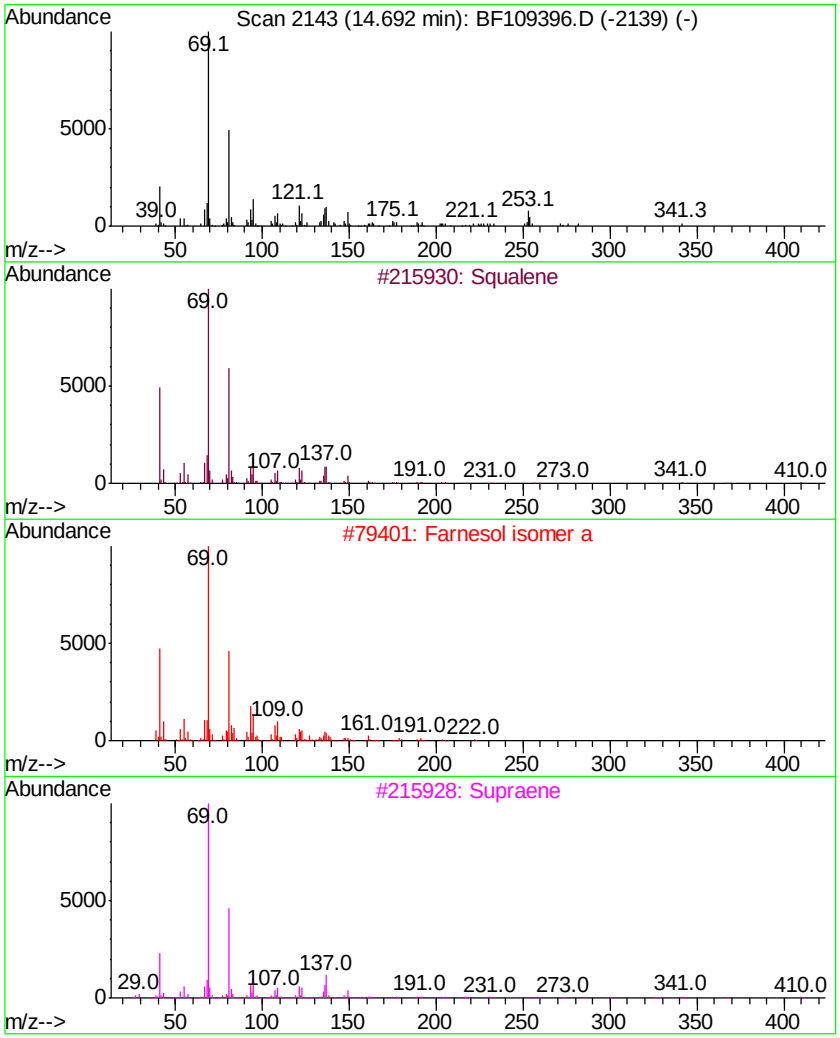
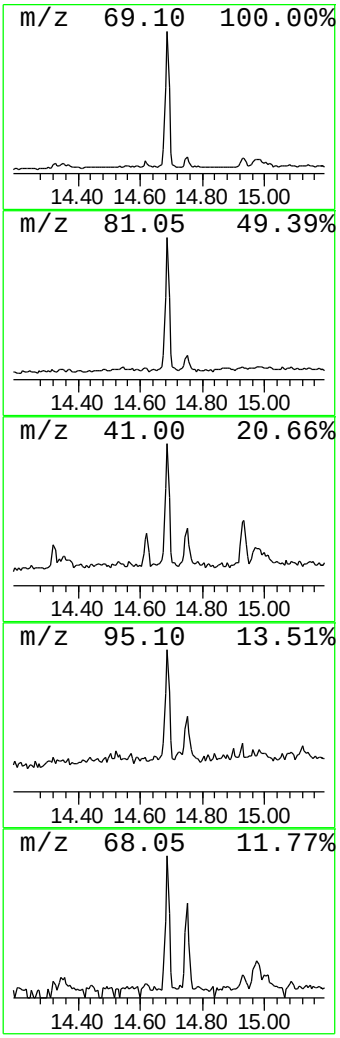
Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	5.03 ng	180517	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Farnesol isomer a	222	C15H26O	1000108-92-4	87
3	Supraene	410	C30H50	007683-64-9	87
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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TIC Library : C:\DATABASE\NIST11.L
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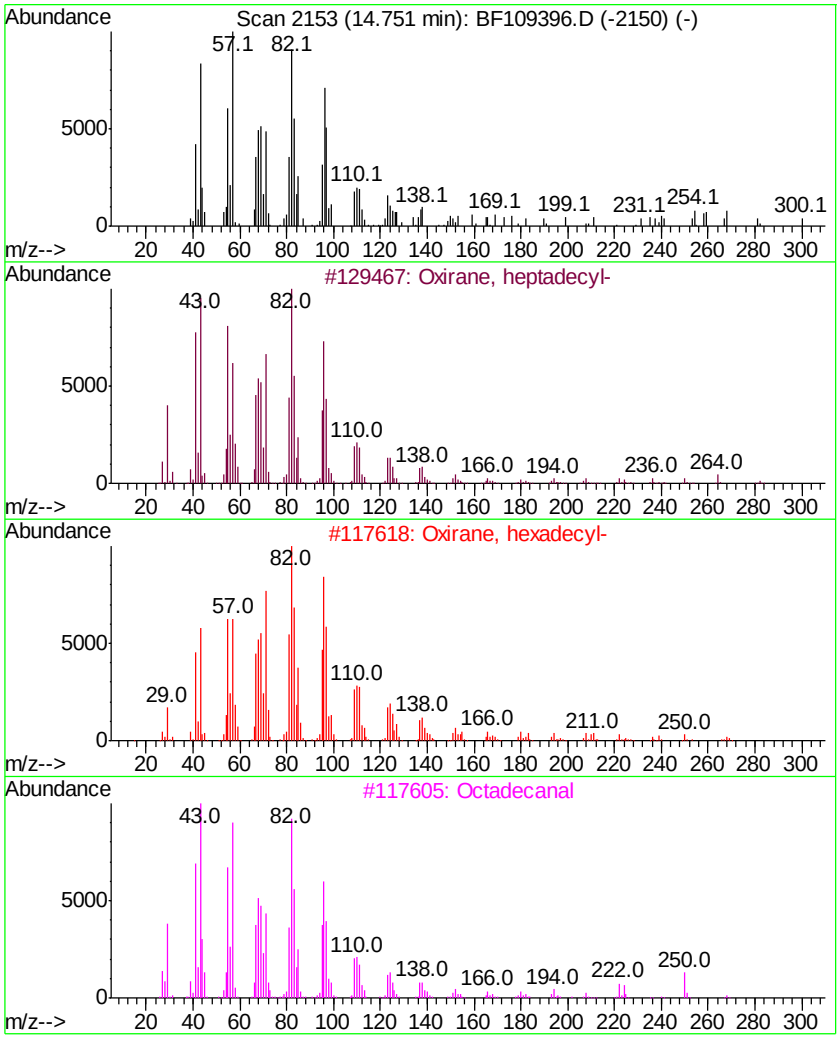
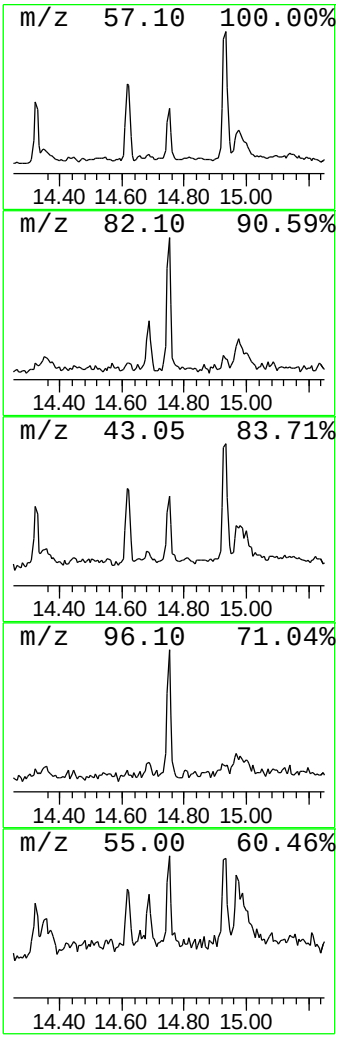
Peak Number 6 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.70 ng	96913	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	97
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Tetradecanal	212	C14H28O	000124-25-4	87
5	Heptadecanal	254	C17H34O	1000376-70-0	83





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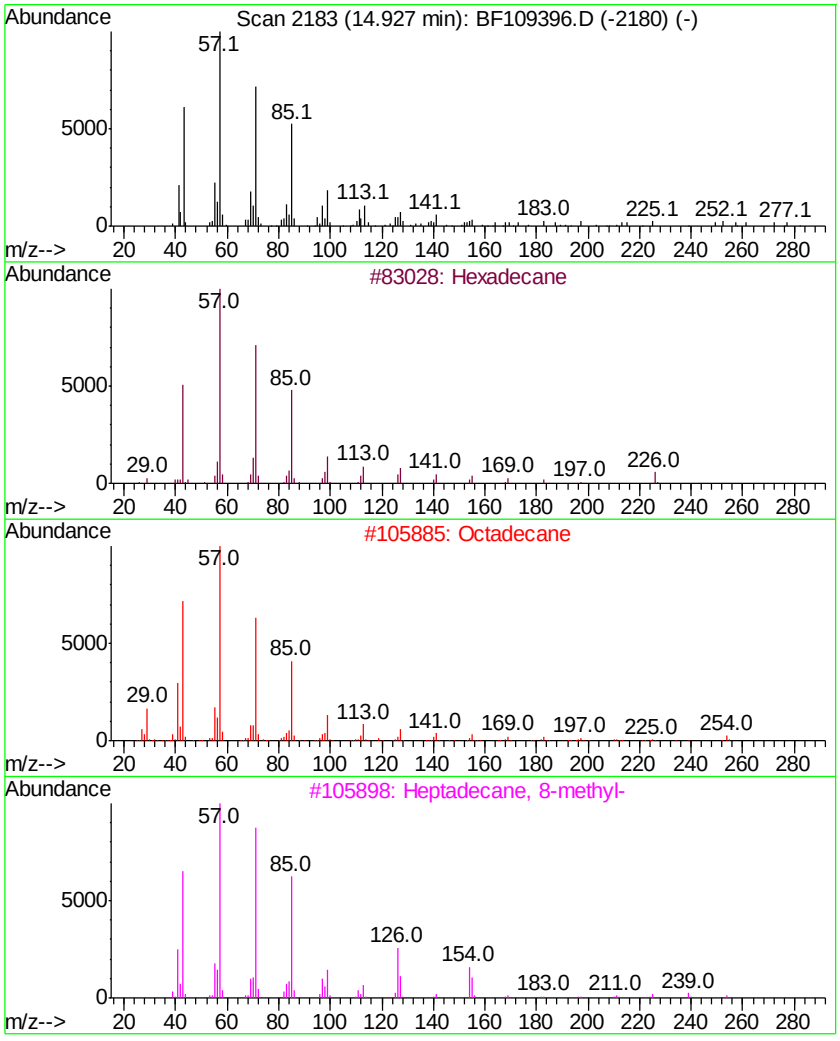
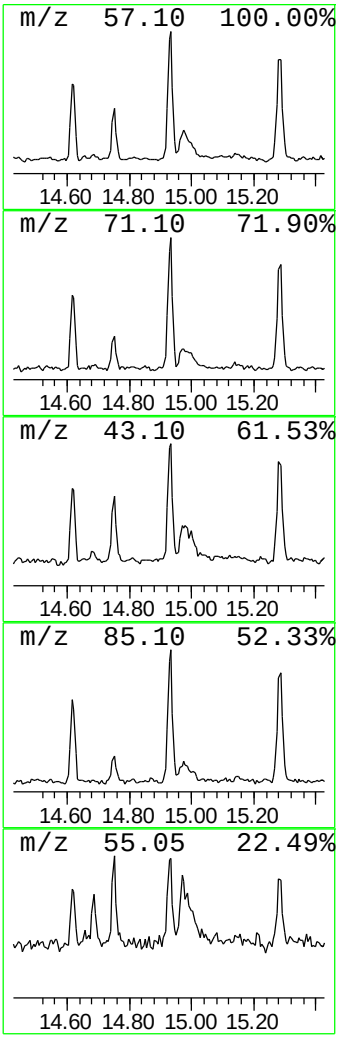
Peak Number 7 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.47 ng	124613	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane	240	C17H36	000629-78-7	90





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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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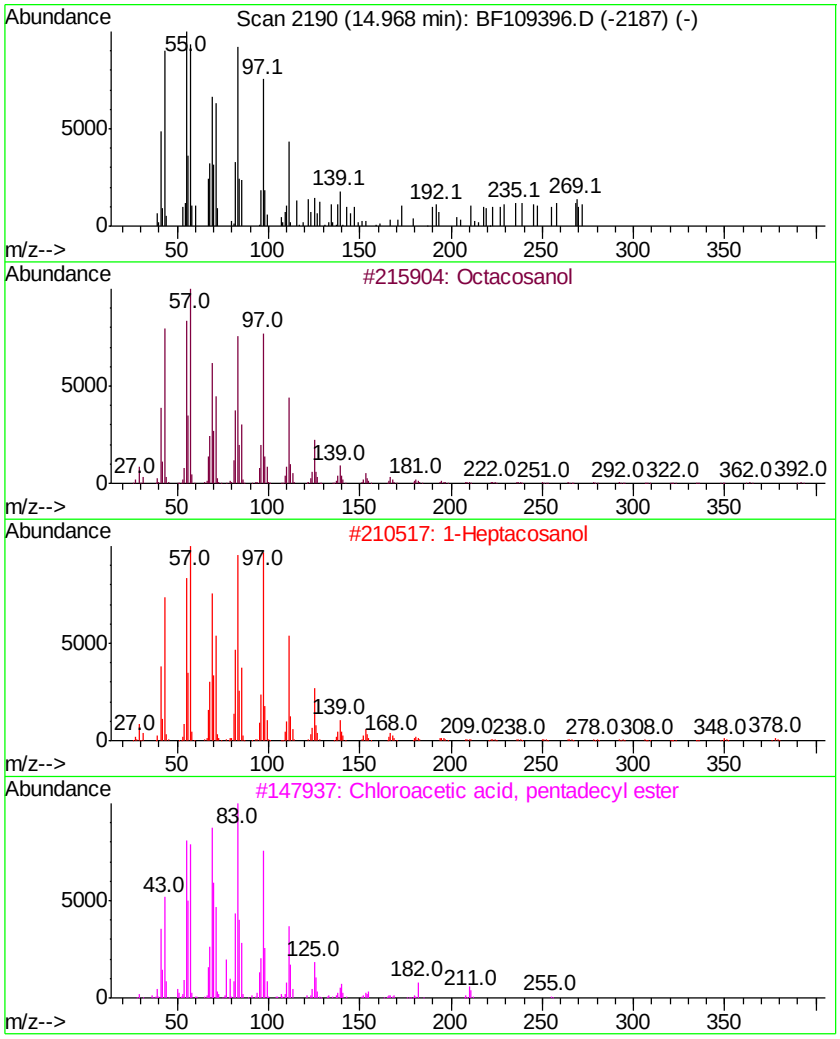
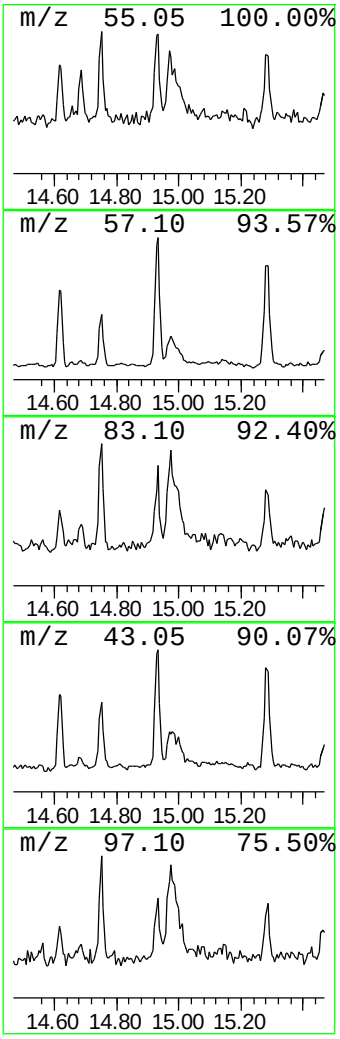
Peak Number 8 Octacosanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.09 ng	75091	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	64
2	1-Heptacosanol	396	C27H56O	002004-39-9	64
3	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	52
4	Cyclohexanone, 3-ethyl-	126	C8H14O	022461-89-8	38
5	1,2,4-Triazole, 5-cyclohexanecar...	194	C9H14N4O	021051-17-2	38





Library Search Compound Report

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Data File : BF109396.D
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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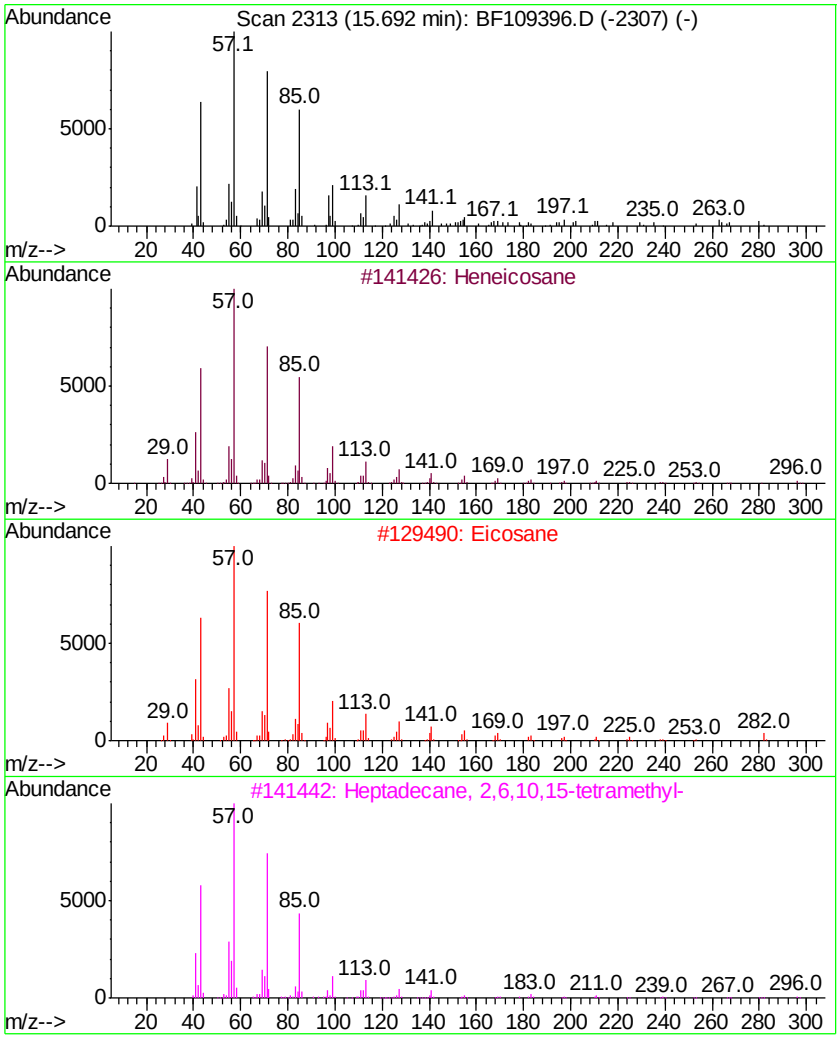
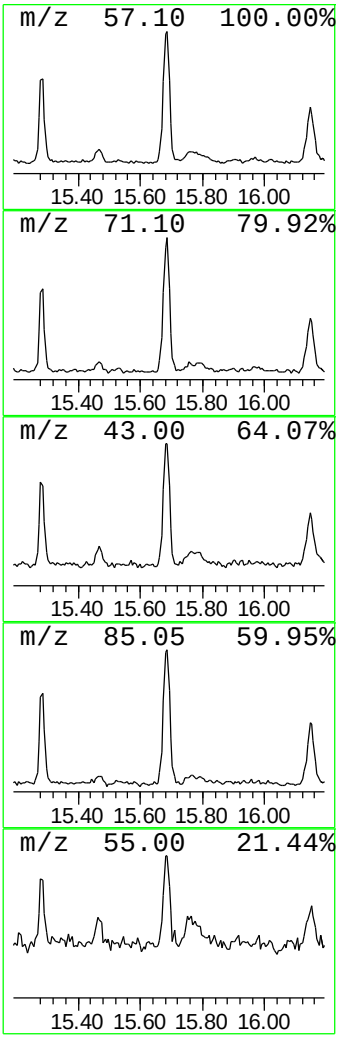
Peak Number 10 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	5.11 ng	183421	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Eicosane	282	C20H42	000112-95-8	97
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109396.D
Acq On : 27 Sep 2018 19:16
Operator : JU/SJ
Sample : J5077-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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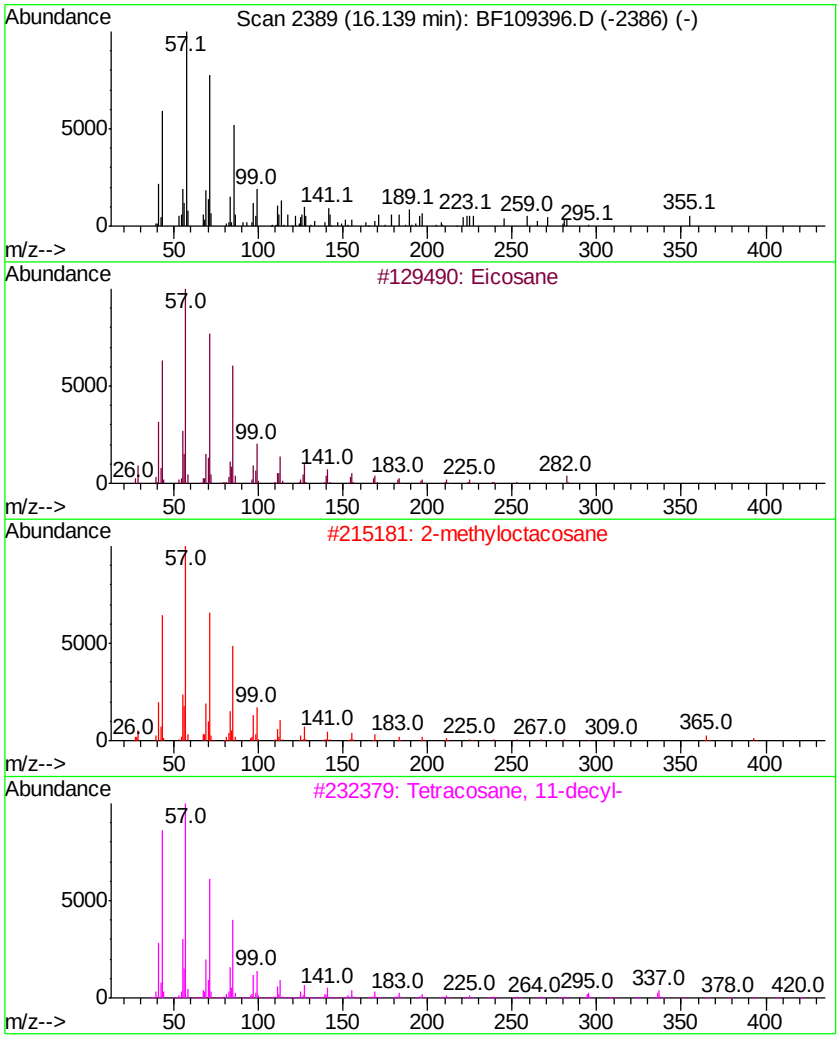
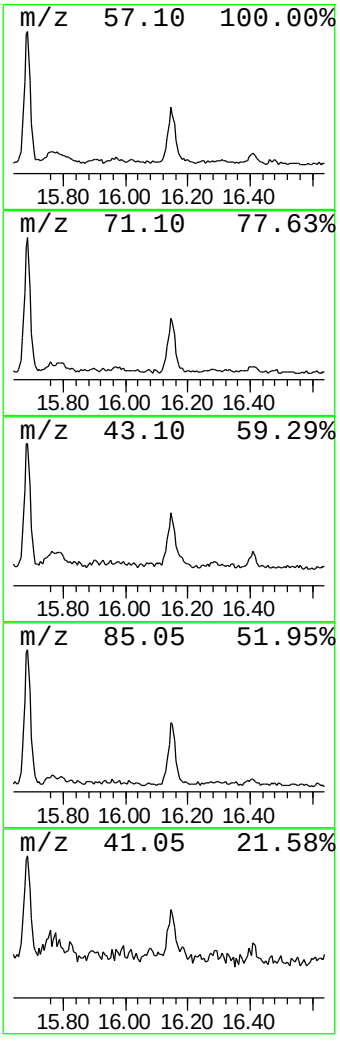
Peak Number 11 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	2.48 ng	89039	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4	Triacontane	422	C30H62	000638-68-6	86
5	Tetracosane	338	C24H50	000646-31-1	86





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Data File : BF109396.D
Acq On : 27 Sep 2018 19:16
Operator : JU/SJ
Sample : J5077-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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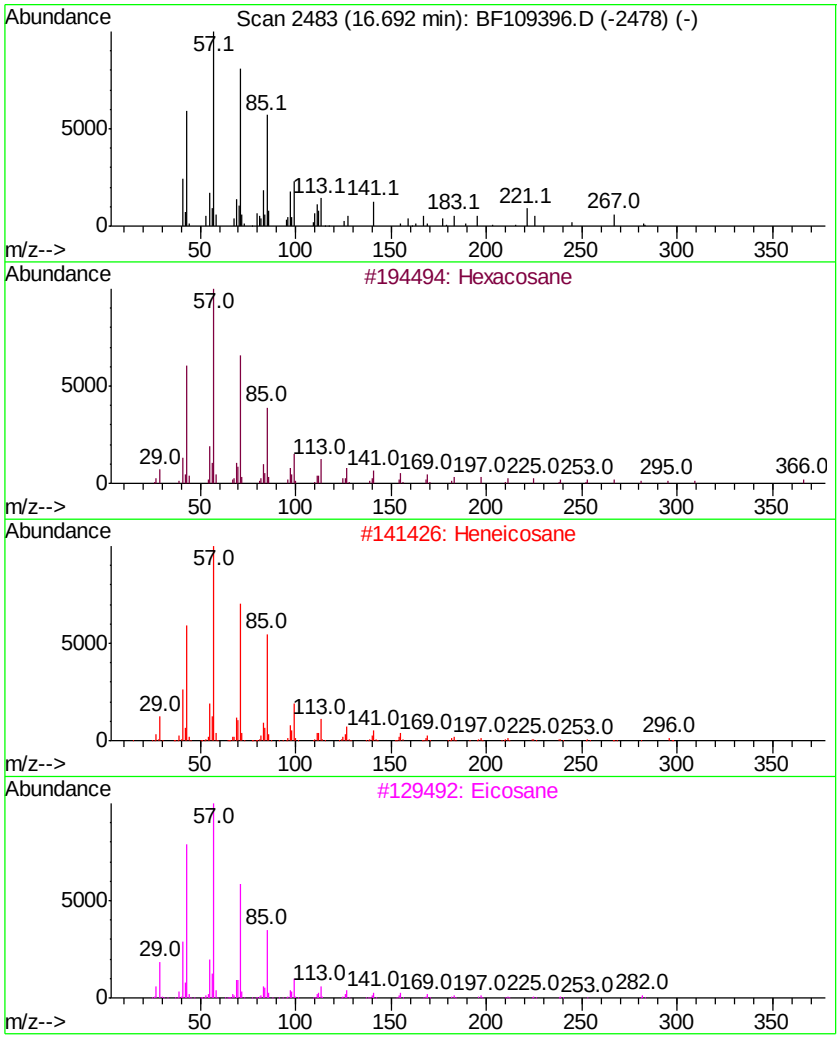
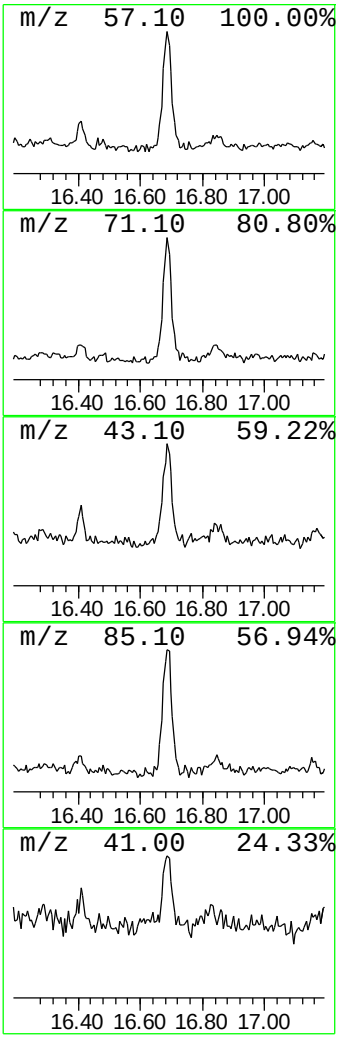
Peak Number 12 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	2.47 ng	88424	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Eicosane	282	C20H42	000112-95-8	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109396.D
Acq On : 27 Sep 2018 19:16
Operator : JU/SJ
Sample : J5077-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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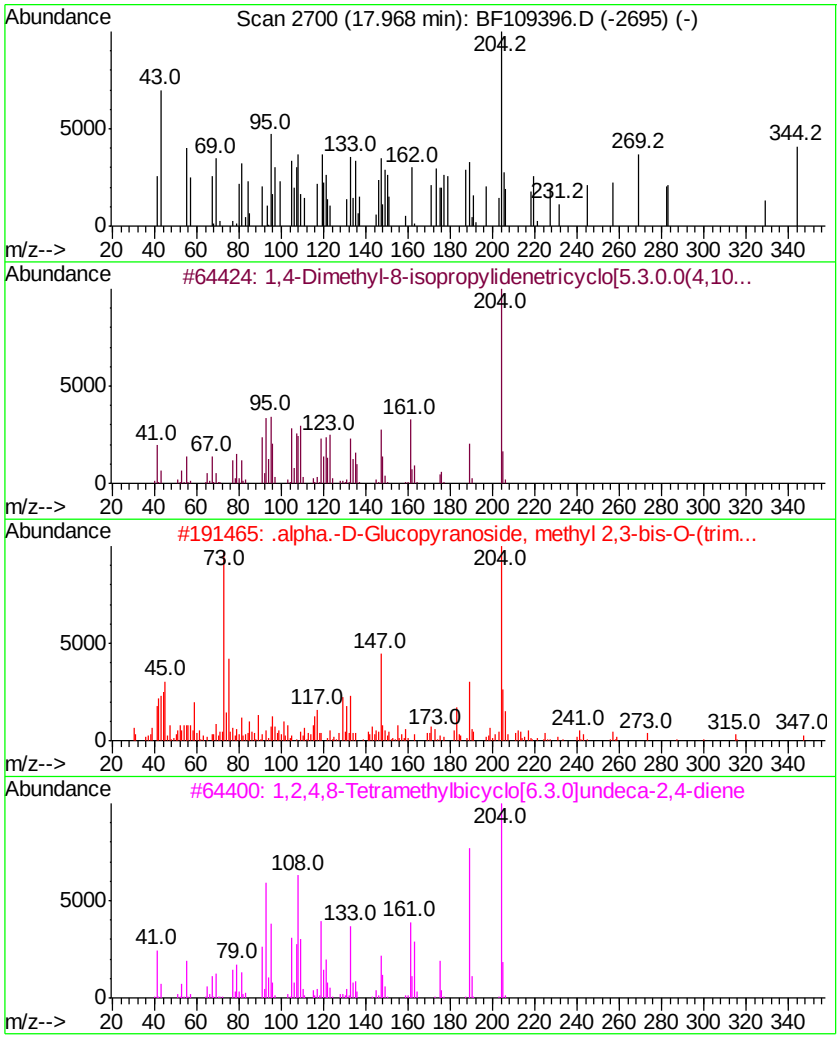
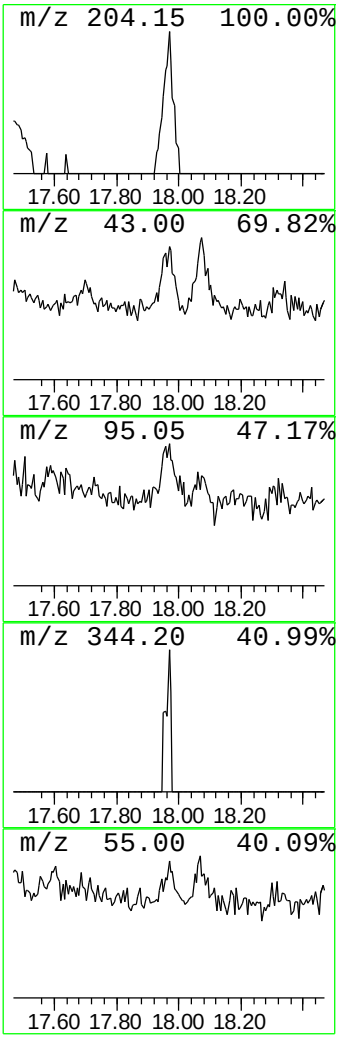
Peak Number 13 unknown17.97 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	2.56 ng	91693	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	27
2	.alpha.-D-Glucopyranoside, methy...	362	C14H31BO6Si2	054400-90-7	22
3	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	16
4	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	15
5	Pyridine-3-carbonitrile, 5-allyl...	204	C11H12N2S	186337-14-4	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109396.D
Acq On : 27 Sep 2018 19:16
Operator : JU/SJ
Sample : J5077-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PARCEL-186-092418-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
unknown6.47	6.47	52.0	ng	1561290	1	6.70	600711	20.0
n-Hexadecanoic acid	11.75	2.4	ng	92276	4	11.21	756765	20.0
Heptadecyl heptaf...	13.71	4.8	ng	200021	5	13.84	828333	20.0
Squalene	14.69	5.0	ng	180517	6	15.24	717254	20.0
Oxirane, heptadecyl-	14.75	2.7	ng	96913	6	15.24	717254	20.0
Hexadecane	14.93	3.5	ng	124613	6	15.24	717254	20.0
Octacosanol	14.97	2.1	ng	75091	6	15.24	717254	20.0
Heneicosane	15.69	5.1	ng	183421	6	15.24	717254	20.0
Eicosane	16.14	2.5	ng	89039	6	15.24	717254	20.0
Hexacosane	16.69	2.5	ng	88424	6	15.24	717254	20.0
unknown17.97	17.97	2.6	ng	91693	6	15.24	717254	20.0