LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112908.D
Acq On : 7 Mar 2019 3:54
Operator : JU/SJ
Sample : K1705-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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	3776455	3690181	89.58%	8.506%
2	6.369	723	728	731	rBV	4005290	4045749	98.21%	9.325%
3	6.498	746	750	754	rBV	4013116	4119452	100.00%	9.495%
4	6.734	786	790	793	rBV	1438303	1299607	31.55%	2.996%
5	6.887	812	816	820	rBV	3668461	3258428	79.10%	7.511%
6	7.287	879	884	892	rBV	2529596	2600178	63.12%	5.993%
7	8.010	1003	1007	1014	rBV	1642570	1573093	38.19%	3.626%
8	8.722	1123	1128	1132	rBV	53337	56091	1.36%	0.129%
9	9.086	1186	1190	1201	rBV	4473742	4050706	98.33%	9.337%
10	9.181	1204	1206	1212	rVB3	40755	46600	1.13%	0.107%
11	9.345	1228	1234	1238	rBV2	38928	80138	1.95%	0.185%
12	9.480	1254	1257	1263	rVB	177678	171750	4.17%	0.396%
13	9.622	1277	1281	1287	rVB	91526	83840	2.04%	0.193%
14	9.763	1301	1305	1309	rBV	1484421	1507705	36.60%	3.475%
15	9.969	1335	1340	1344	rBV3	36157	45704	1.11%	0.105%
16	10.545	1433	1438	1449	rBV	2363195	2364922	57.41%	5.451%
17	11.239	1552	1556	1558	rBV	1284830	1313513	31.89%	3.028%
18	11.257	1558	1559	1564	rVV	291253	245646	5.96%	0.566%
19	11.310	1566	1568	1571	rVB	67773	61170	1.48%	0.141%
20	11.704	1631	1635	1638	rBV5	29145	53679	1.30%	0.124%
21	11.739	1638	1641	1643	rBV	66805	64089	1.56%	0.148%
22	11.774	1643	1647	1651	rBV2	540125	562480	13.65%	1.296%
23	11.845	1656	1659	1662	rVV2	101204	137480	3.34%	0.317%
24	11.869	1662	1663	1668	rVB	71154	55297	1.34%	0.127%
25	12.051	1692	1694	1700	rVB3	39018	54186	1.32%	0.125%
26	12.286	1728	1734	1737	rBV	83886	110102	2.67%	0.254%
27	12.322	1737	1740	1742	rVV2	52654	73655	1.79%	0.170%
28	12.369	1745	1748	1752	rVB4	37617	57541	1.40%	0.133%
29	12.439	1757	1760	1764	rBV	315265	299453	7.27%	0.690%
30	12.498	1764	1770	1774	rVB7	39798	86722	2.11%	0.200%
31	12.557	1777	1780	1788	rVV3	173928	215071	5.22%	0.496%
32	12.669	1794	1799	1802	rBV	334510	363044	8.81%	0.837%
33	12.816	1820	1824	1828	rBV	3267408	2970917	72.12%	6.848%
34	12.886	1833	1836	1839	rBV3	39367	47531	1.15%	0.110%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112908.D
Acq On : 7 Mar 2019 3:54
Operator : JU/SJ
Sample : K1705-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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	12.992	1848	1854	1858	rVB2	73123	142700	3.46%	0.329%
36	13.063	1863	1866	1869	rVB	74610	65075	1.58%	0.150%
37	13.098	1869	1872	1875	rBV2	73805	80829	1.96%	0.186%
38	13.221	1890	1893	1898	rVB	54396	55232	1.34%	0.127%
39	13.304	1904	1907	1913	rVB4	98478	101005	2.45%	0.233%
40	13.404	1921	1924	1929	rVB2	74971	80926	1.96%	0.187%
41	13.498	1937	1940	1945	rVB	57140	85514	2.08%	0.197%
42	13.610	1955	1959	1962	rBV3	37525	54989	1.33%	0.127%
43	13.727	1973	1979	1986	rBV2	368159	494948	12.01%	1.141%
44	13.857	1996	2001	2004	rBV	1519365	1751020	42.51%	4.036%
45	13.886	2004	2006	2012	rVB	200448	188846	4.58%	0.435%
46	14.045	2030	2033	2037	rVB	219159	202035	4.90%	0.466%
47	14.245	2065	2067	2070	rVB	62089	51883	1.26%	0.120%
48	14.351	2081	2085	2095	rVB4	350290	612510	14.87%	1.412%
49	14.639	2131	2134	2141	rVB	353334	381176	9.25%	0.879%
50	14.774	2155	2157	2161	rVB2	65381	70751	1.72%	0.163%
51	14.868	2169	2173	2183	rVB	146915	271796	6.60%	0.626%
52	14.957	2185	2188	2192	rBV2	422942	486131	11.80%	1.121%
53	15.145	2218	2220	2224	rVB	98088	98318	2.39%	0.227%
54	15.204	2227	2230	2234	rVB	136425	152787	3.71%	0.352%
55	15.262	2236	2240	2245	rVV	931420	1210574	29.39%	2.790%
56	15.315	2245	2249	2253	rVB	286493	366723	8.90%	0.845%
57	15.715	2313	2317	2321	rBV	267544	375441	9.11%	0.865%
58	16.186	2393	2397	2407	rVB2	129457	237881	5.77%	0.548%

Sum of corrected areas: 43384810

LSC Report - Integrated Chromatogram

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Sample : K1705-12
Misc :
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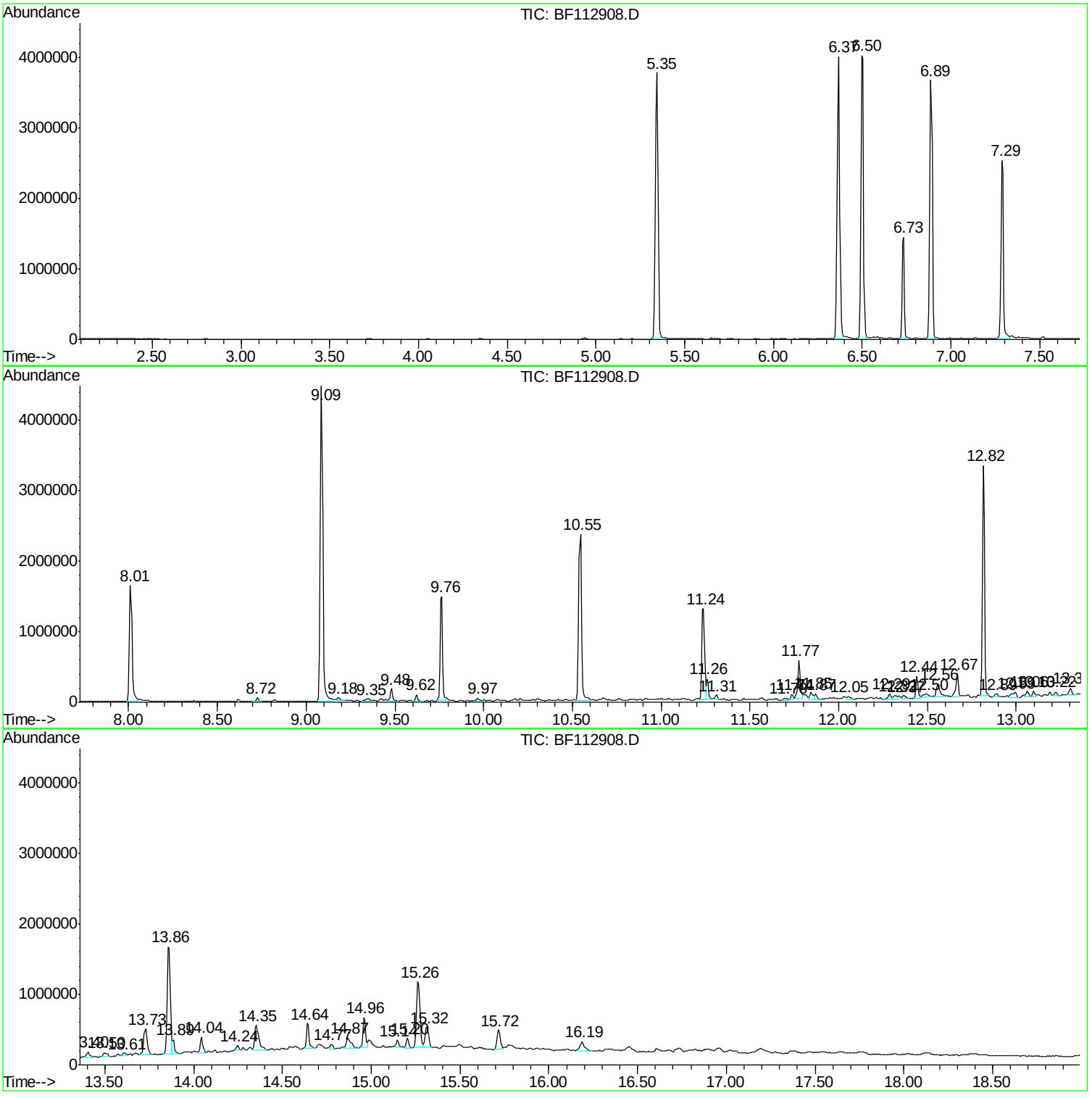
Instrument :
BNA_F
ClientSampleId :
EXT-027-SW014-022719

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 : BF112908.D
Acq On : 7 Mar 2019 3:54
Operator : JU/SJ
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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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

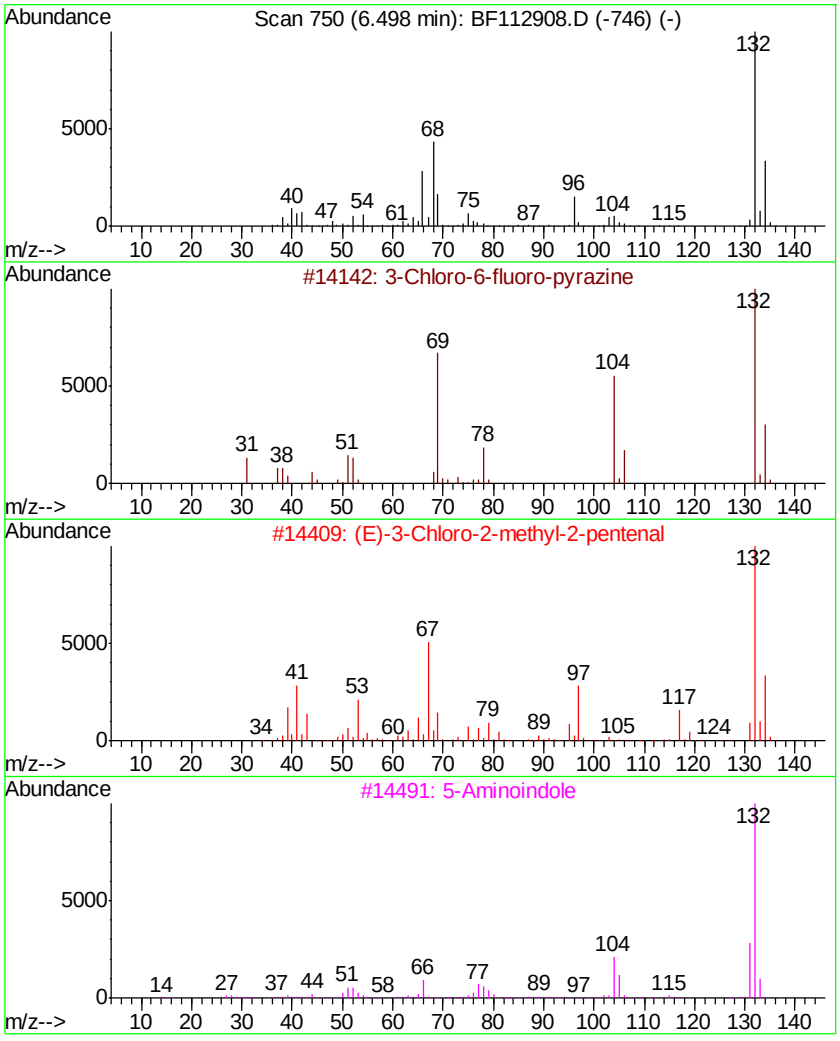
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

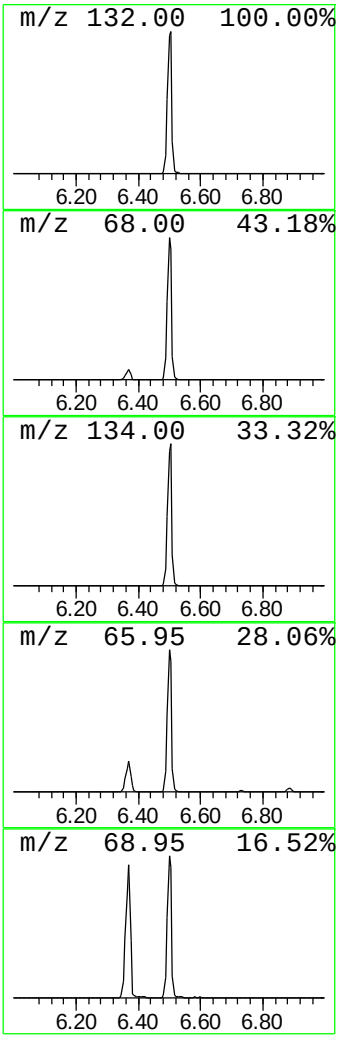
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	63.40 ng	4119450	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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Amphetaminil	250	C17H18N2	017590-01-1	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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Operator : JU/SJ
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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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

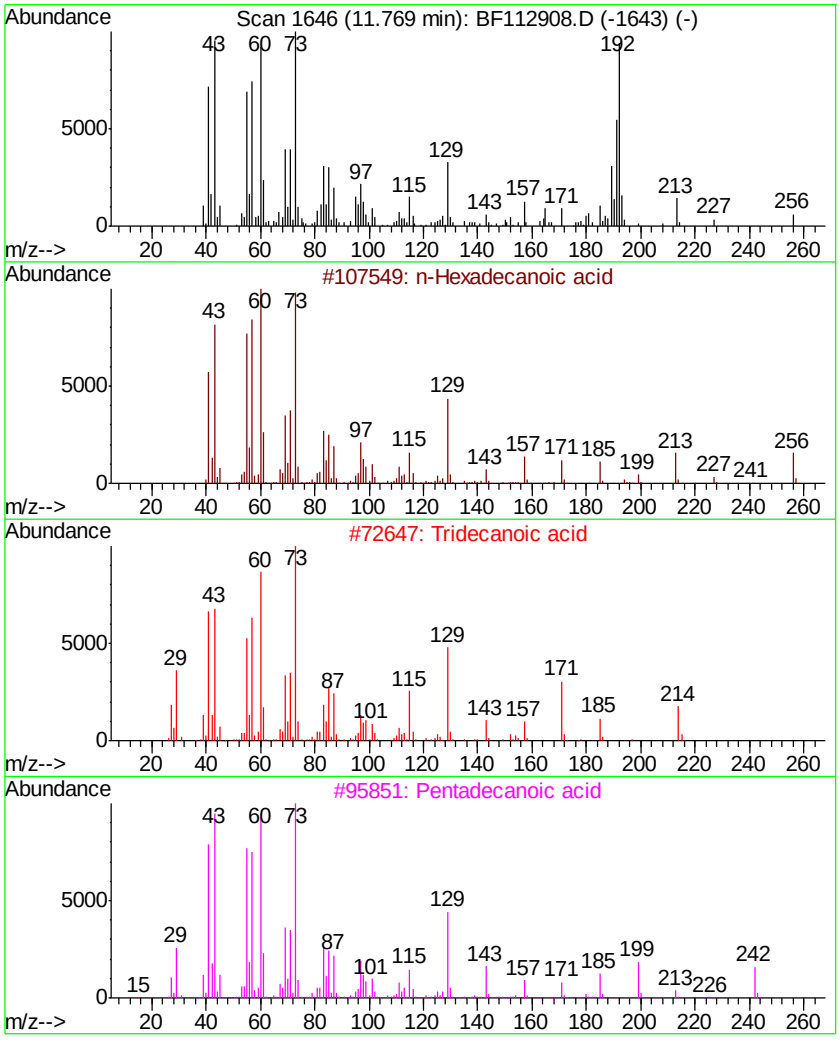
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

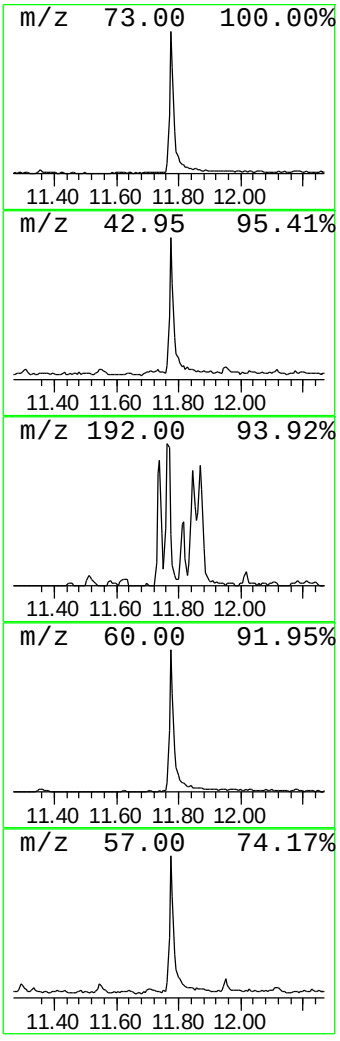
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	8.56 ng	562480	Phenanthrene-d10	11.24

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	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112908.D
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Operator : JU/SJ
Sample : K1705-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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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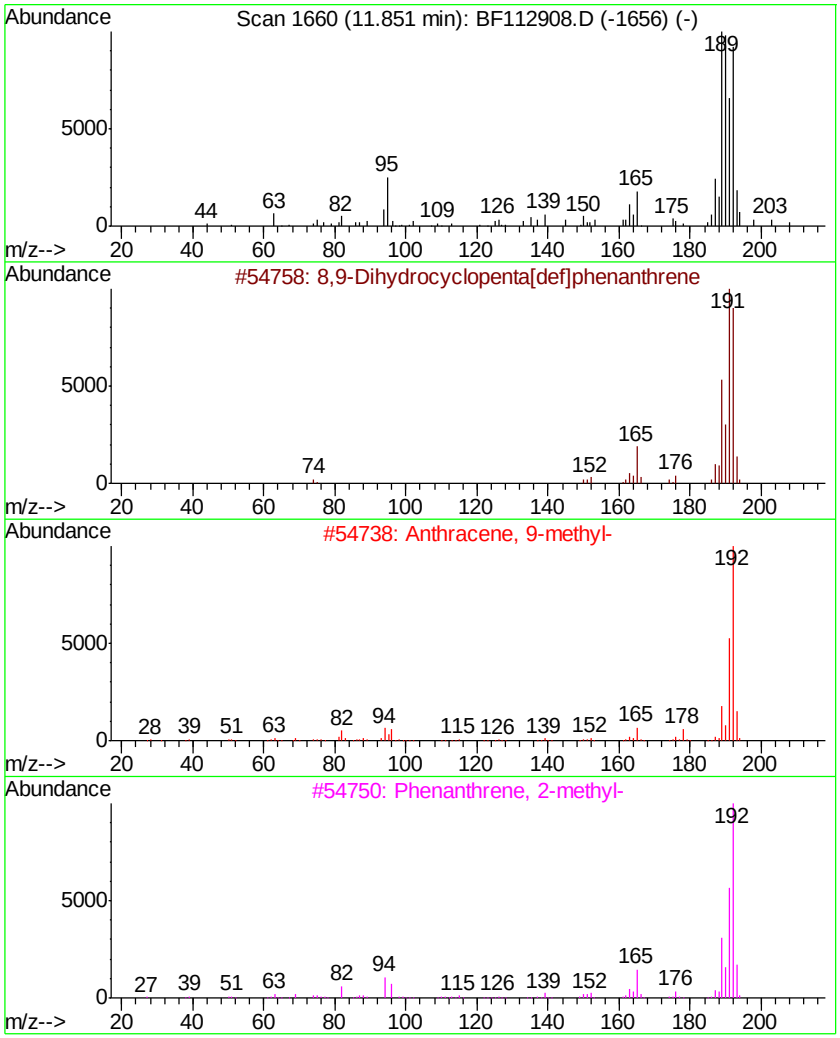
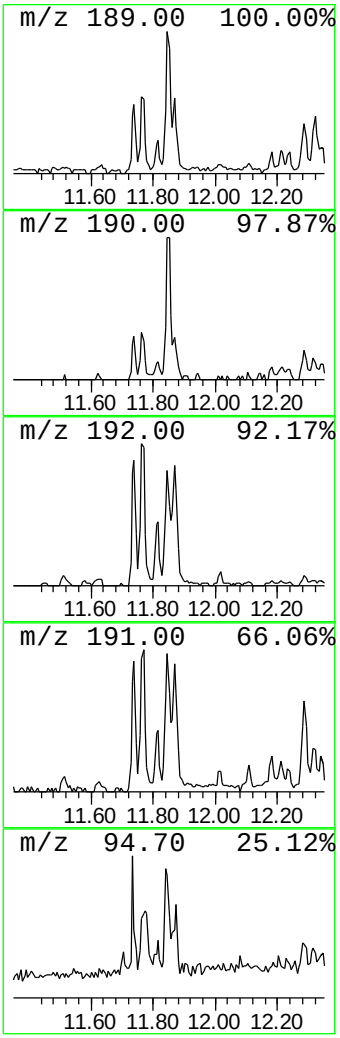
Peak Number 4 8,9-Dihydrocyclopenta[def]p... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.09 ng	137480	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	80
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	49
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	46
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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Acq On : 7 Mar 2019 3:54
Operator : JU/SJ
Sample : K1705-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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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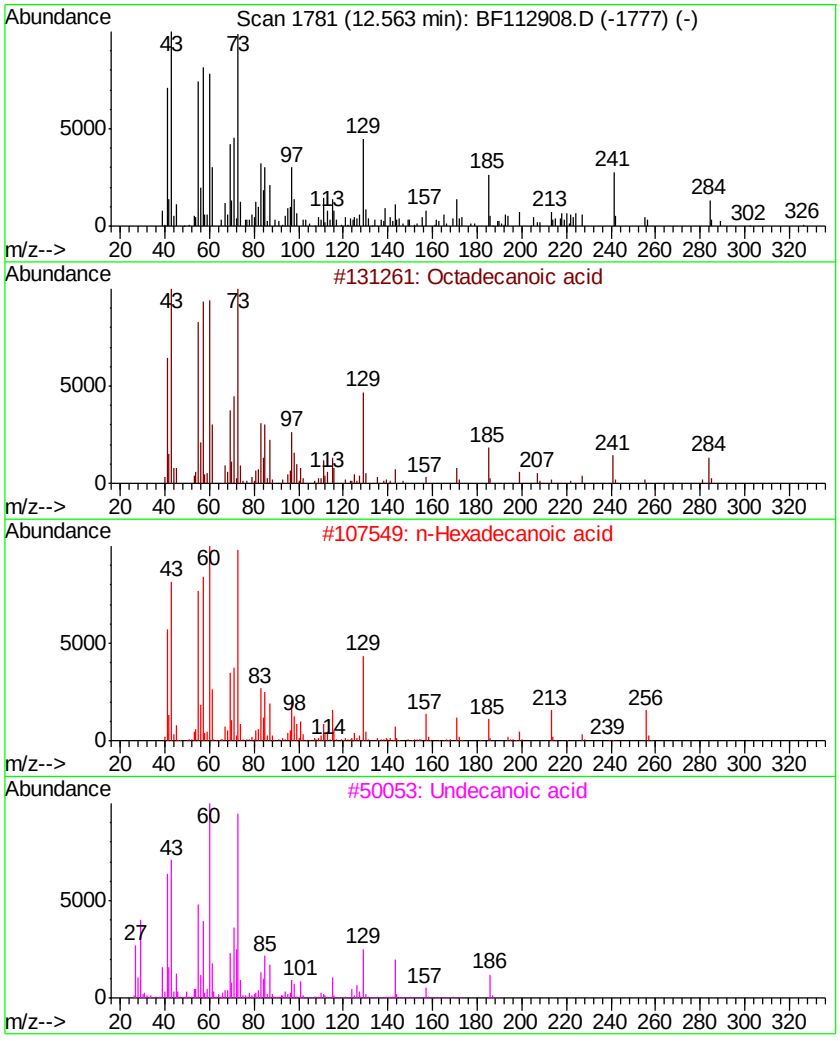
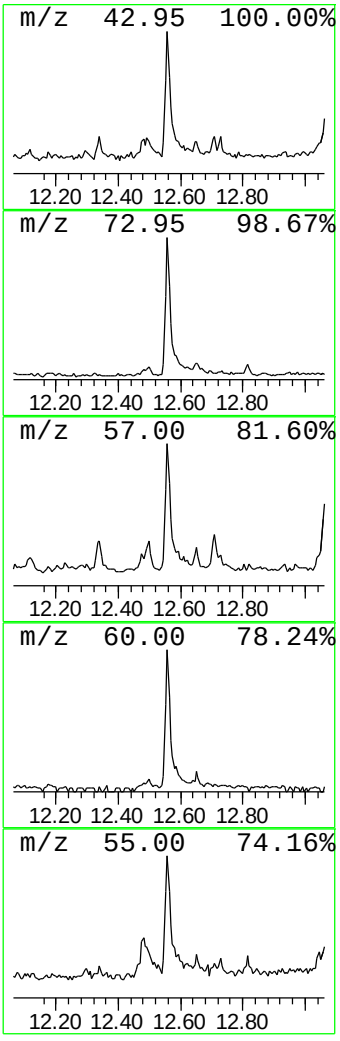
Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.46 ng	215071	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Misc :
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Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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

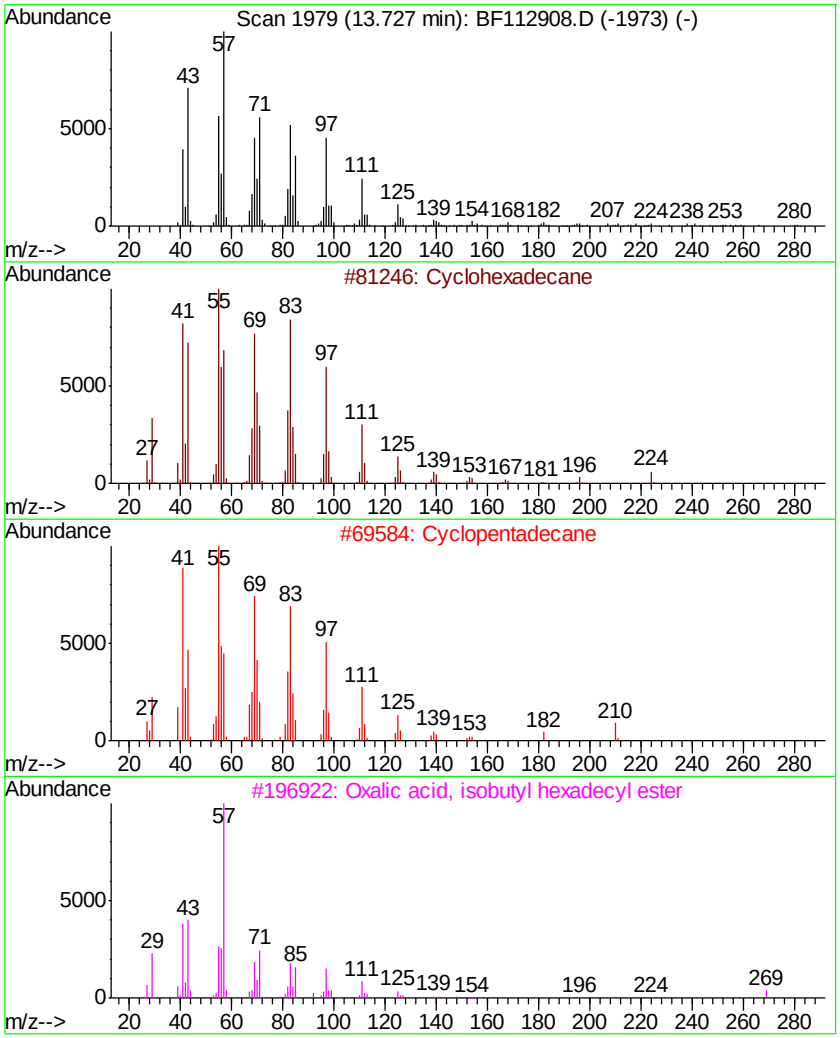
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

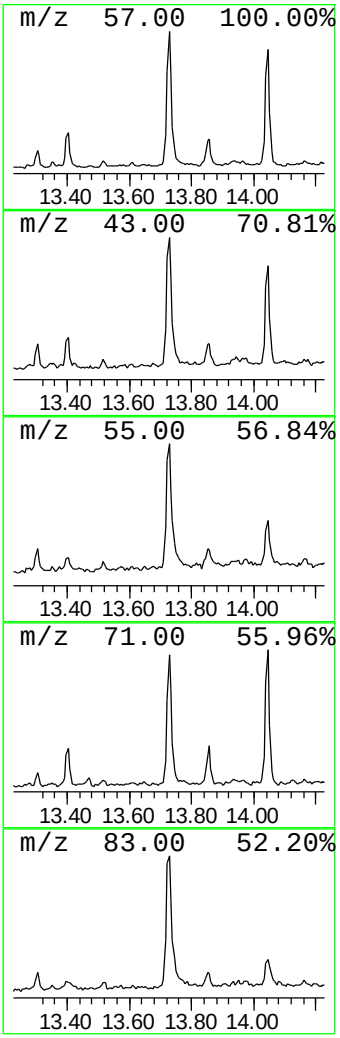
****

Peak Number 6 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	5.65 ng	494948	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91





Library Search Compound Report

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

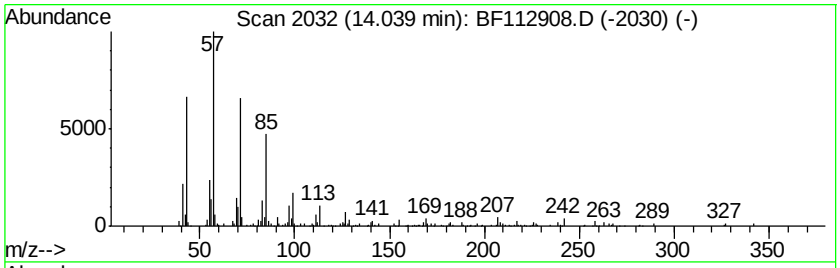
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

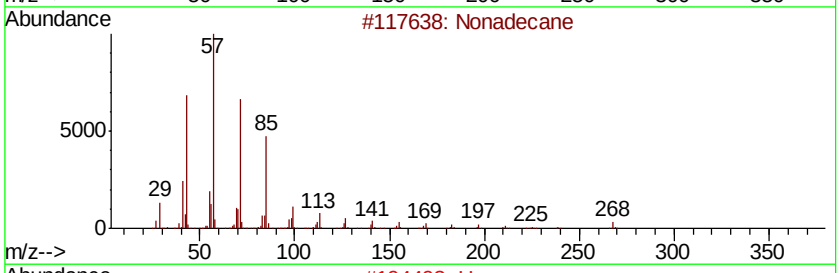
****

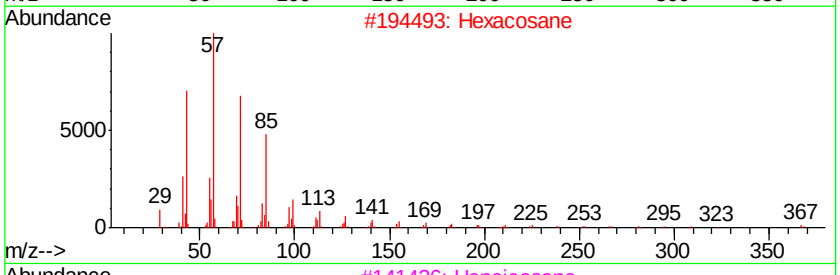
Peak Number 7 Nonadecane Concentration Rank 12

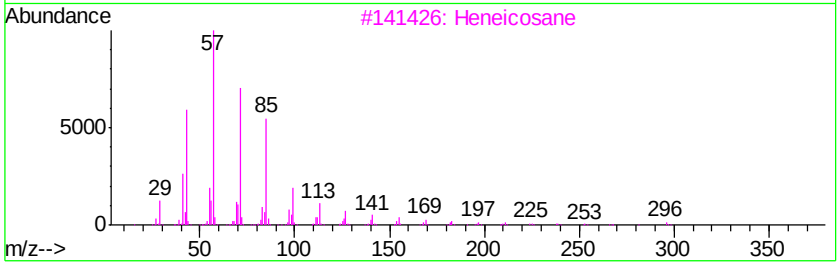
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.31 ng	202035	Chrysene-d12	13.86

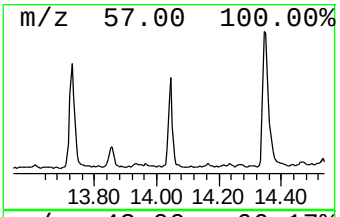
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane	296	C21H44	000629-94-7	83
4	Heptadecane	240	C17H36	000629-78-7	83
5	Tetratetracontane	619	C44H90	007098-22-8	76

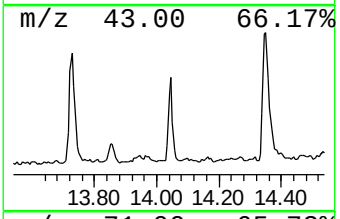


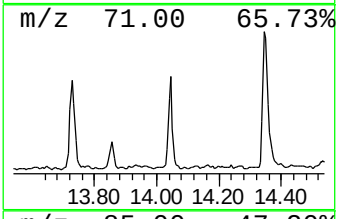


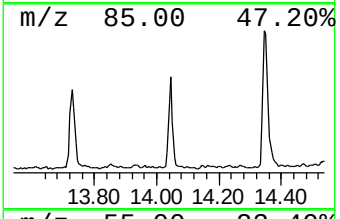


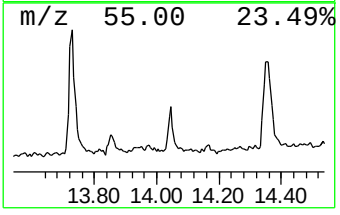












Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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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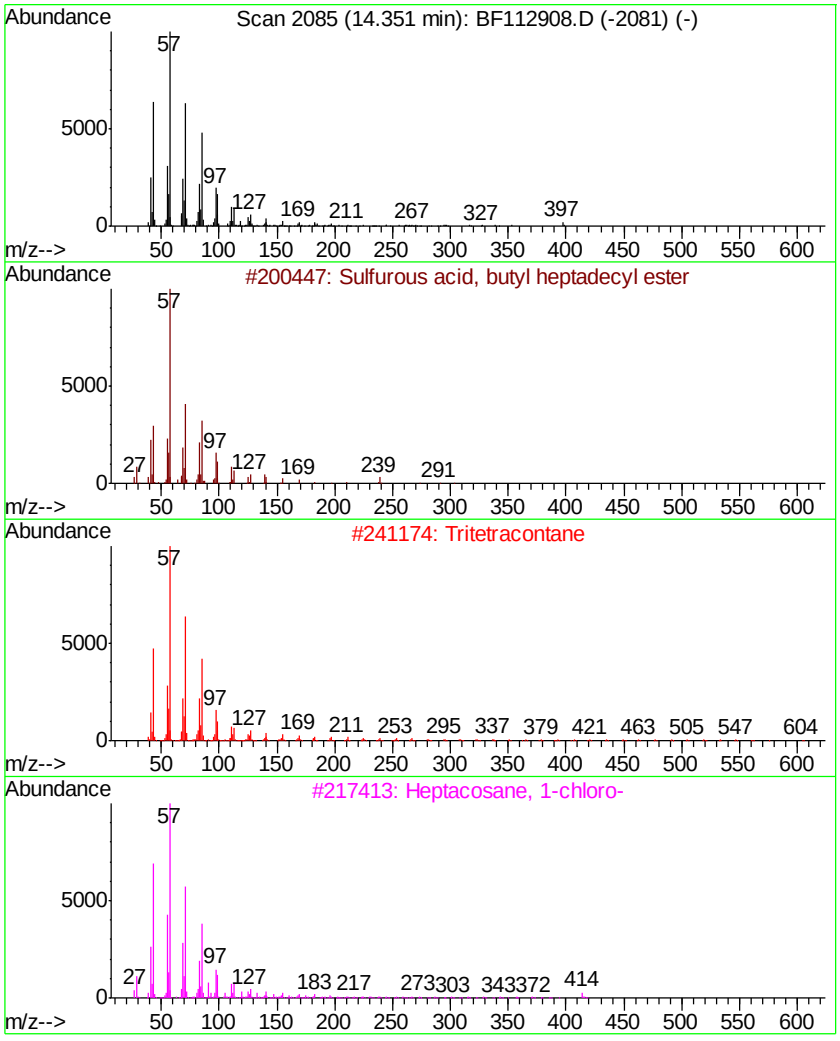
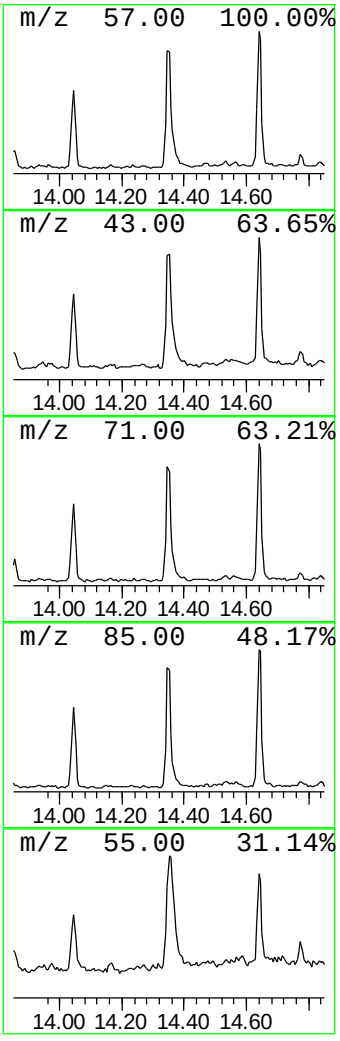
Peak Number 8 Sulfurous acid, butyl hepta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	7.00 ng	612510	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2	Tritetracontane	605	C43H88	007098-21-7	91
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91





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Acq On : 7 Mar 2019 3:54
Operator : JU/SJ
Sample : K1705-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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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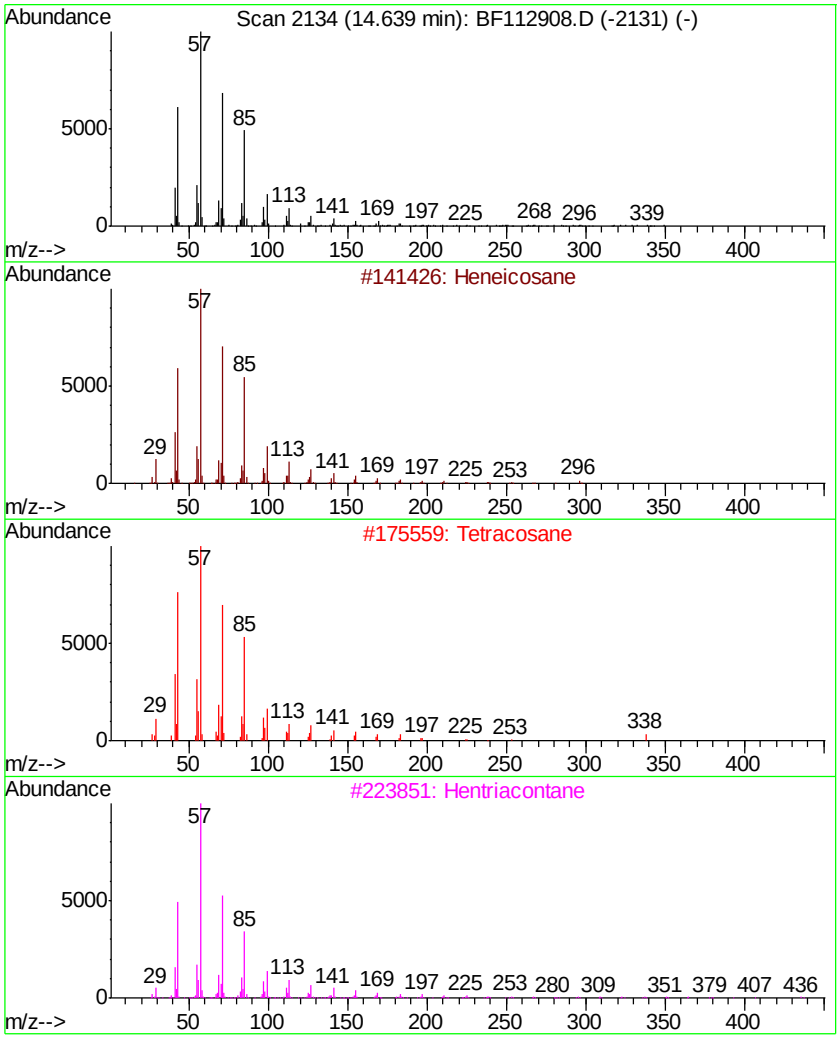
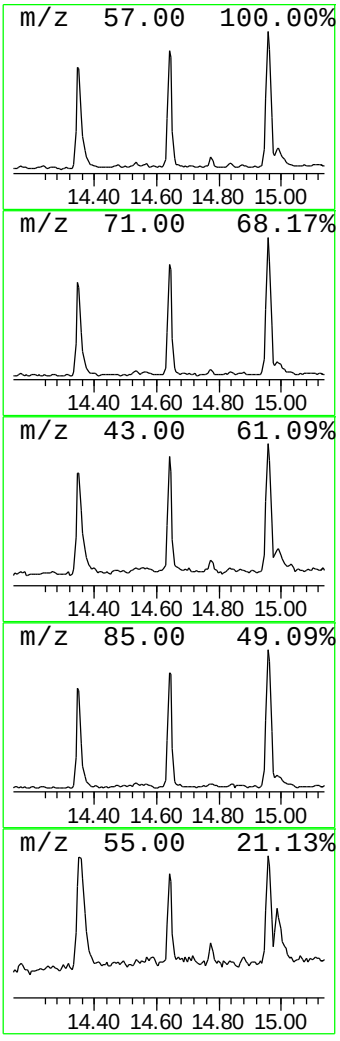
Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	6.30 ng	381176	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Tetracosane	338	C24H50	000646-31-1	91
3	Hentriacontane	437	C31H64	000630-04-6	86
4	Nonadecane	268	C19H40	000629-92-5	86
5	Heptacosane	380	C27H56	000593-49-7	83





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Sample : K1705-12
Misc :
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Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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TIC Integration Parameters: LSCINT.P

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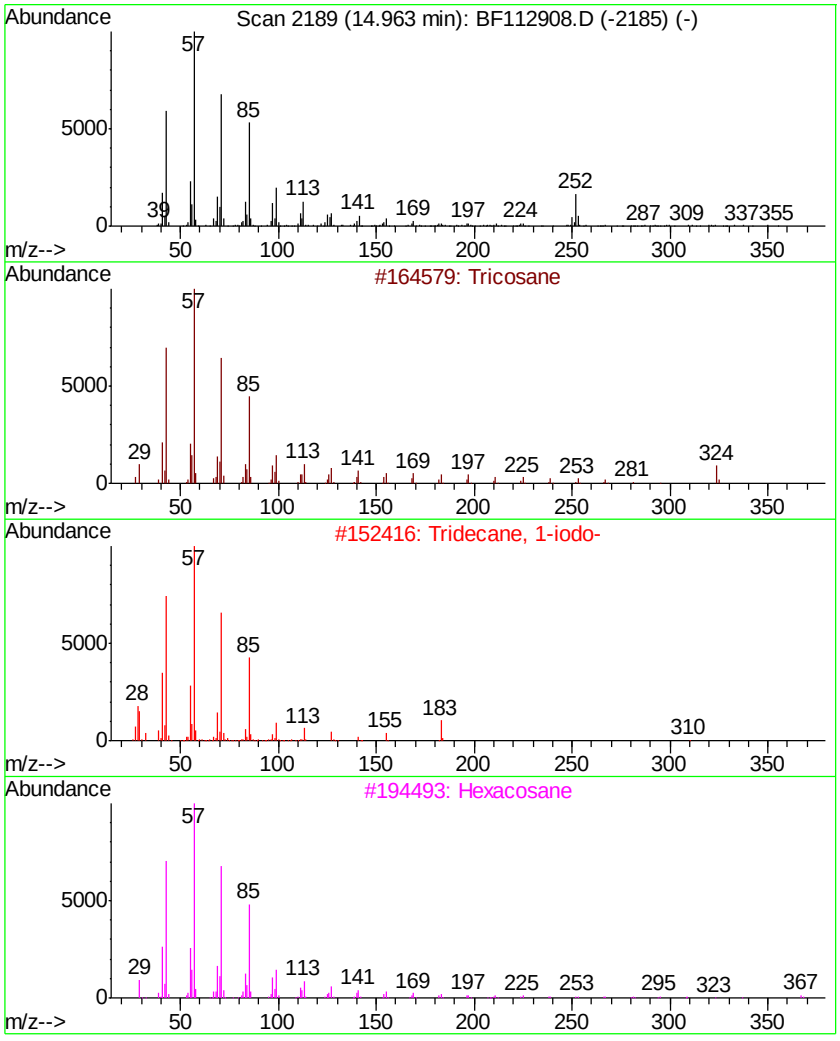
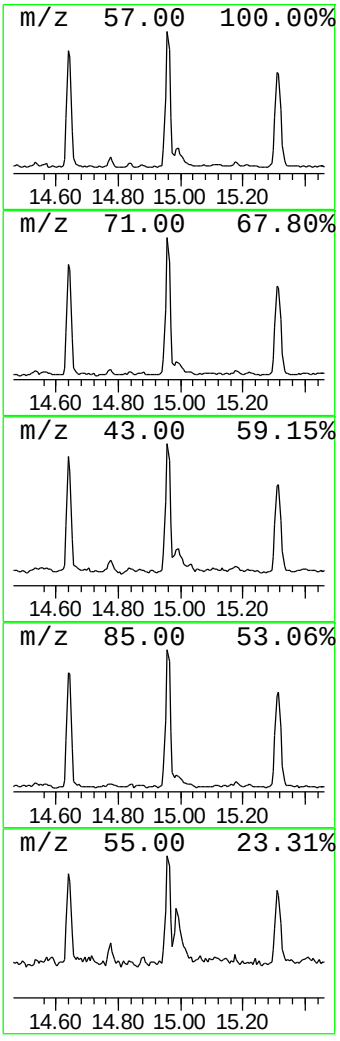
Peak Number 10 Tricosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	8.03 ng	486131	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	94
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87





Library Search Compound Report

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Data File : BF112908.D
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Operator : JU/SJ
Sample : K1705-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-027-SW014-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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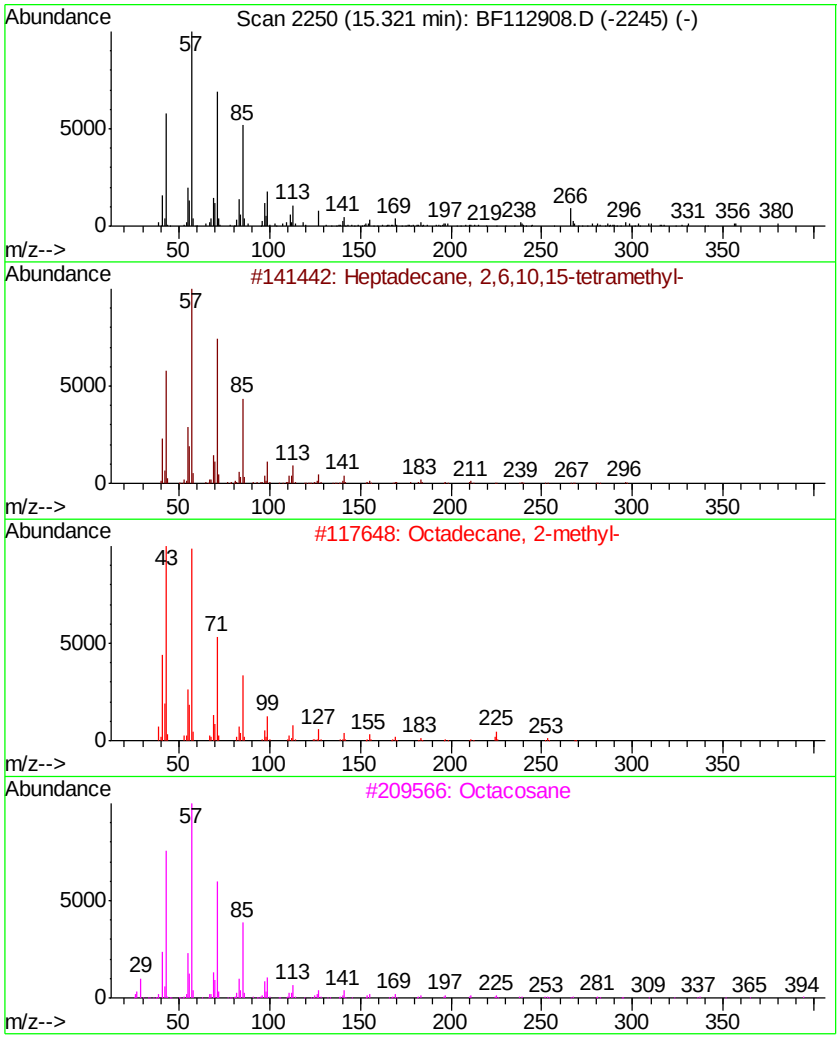
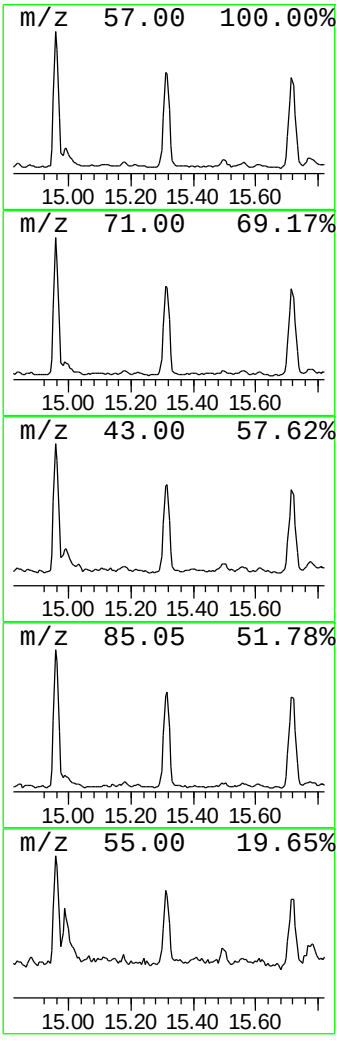
Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	6.06 ng	366723	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
3	Octacosane	394	C28H58	000630-02-4	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Tricosane	324	C23H48	000638-67-5	87





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

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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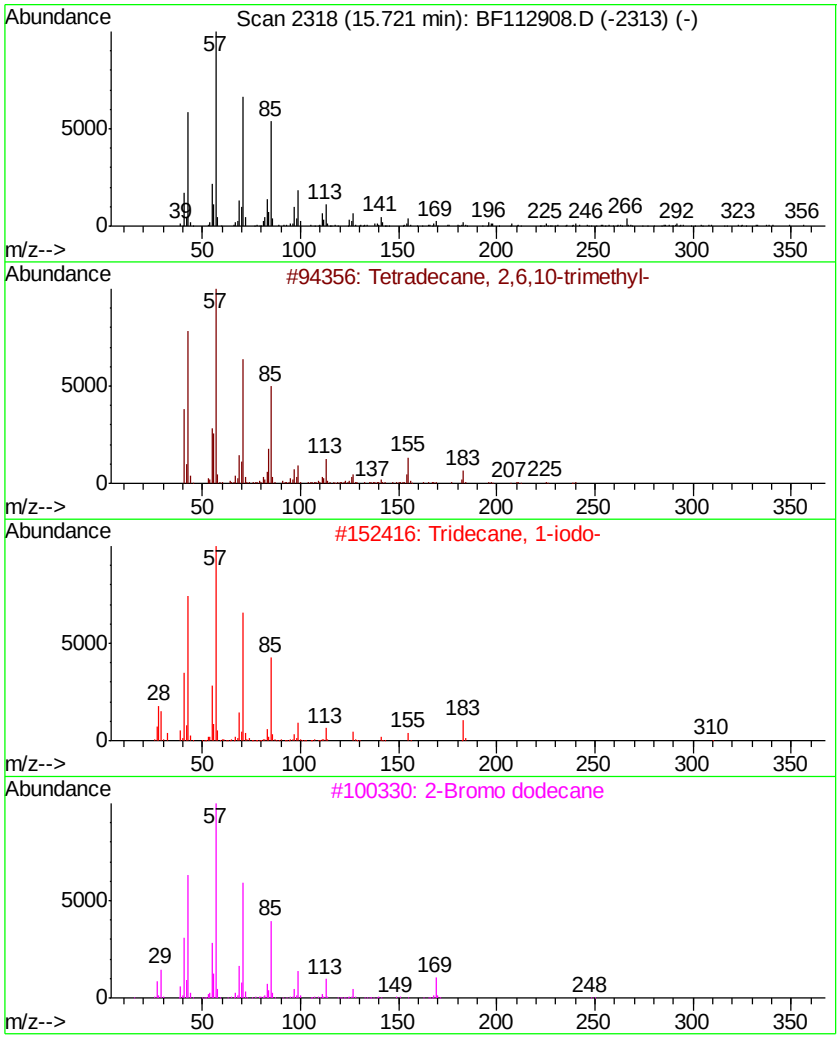
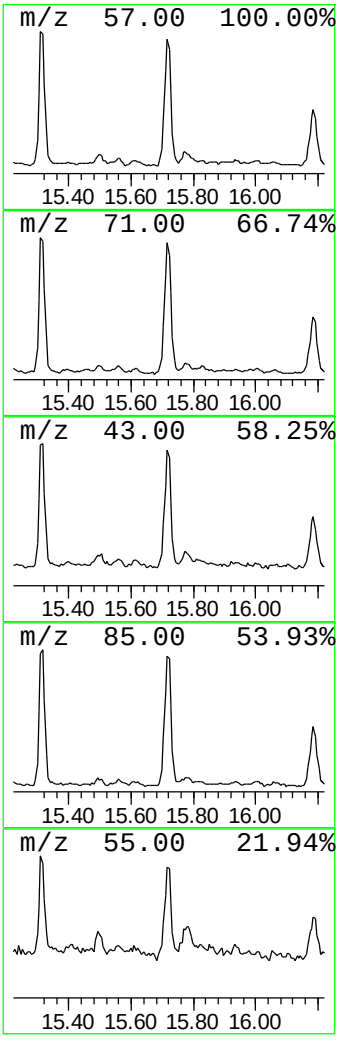
Peak Number 12 Tetradecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	6.20 ng	375441	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Library Search Compound Report

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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-027-SW014-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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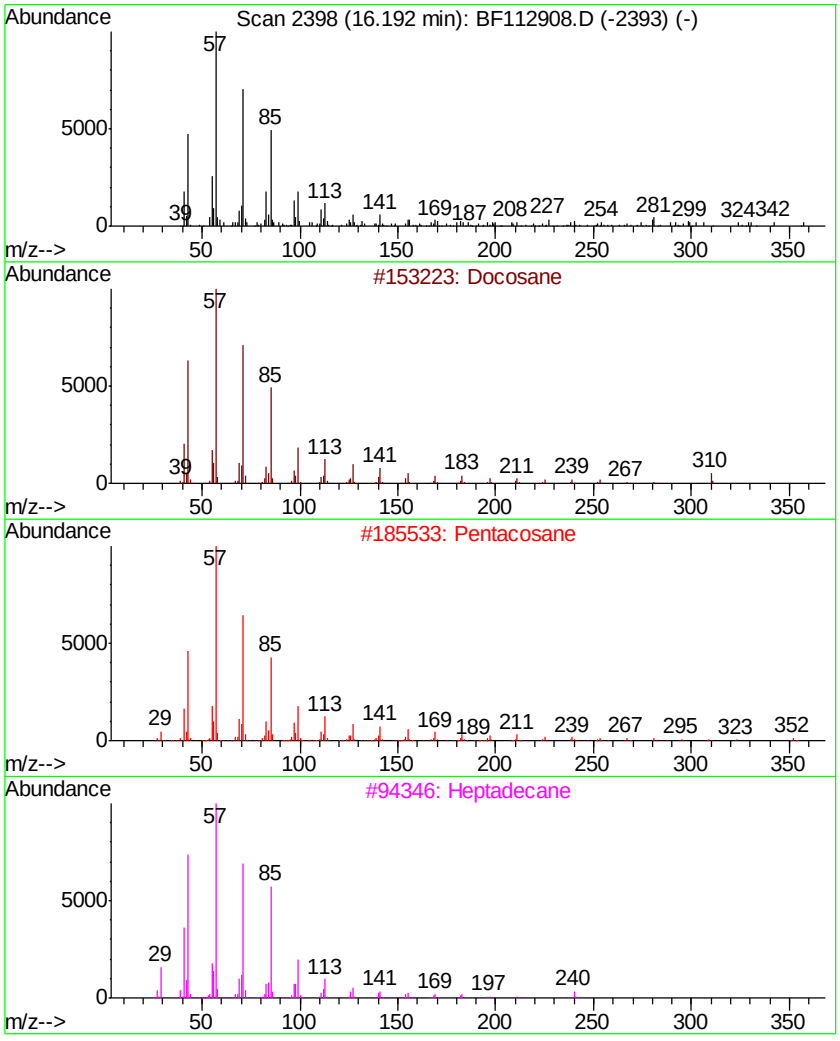
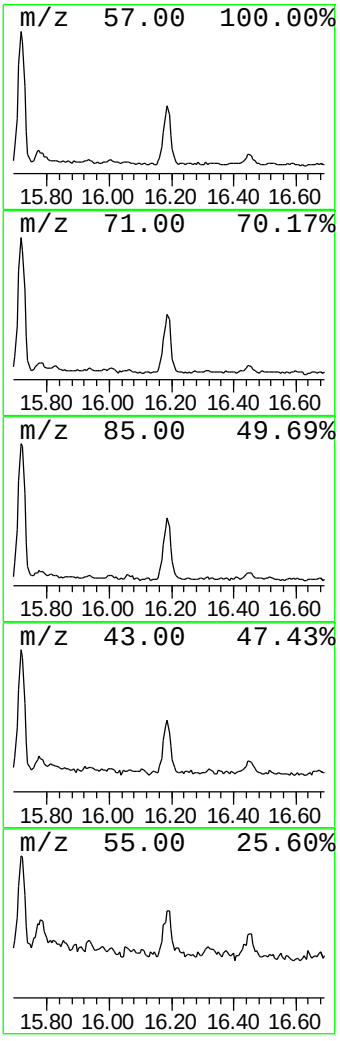
Peak Number 13 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	3.93 ng	237881	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	95
2	Pentacosane	352	C25H52	000629-99-2	95
3	Heptadecane	240	C17H36	000629-78-7	93
4	Octadecane	254	C18H38	000593-45-3	91
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030619\
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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	63.4	ng	4119450	1	6.73	1299610	20.0
n-Hexadecanoic acid	11.77	8.6	ng	562480	4	11.24	1313510	20.0
8,9-Dihydrocyclop...	11.85	2.1	ng	137480	4	11.24	1313510	20.0
Octadecanoic acid	12.56	2.5	ng	215071	5	13.86	1751020	20.0
Cyclohexadecane	13.73	5.7	ng	494948	5	13.86	1751020	20.0
Nonadecane	14.04	2.3	ng	202035	5	13.86	1751020	20.0
Sulfurous acid, b...	14.35	7.0	ng	612510	5	13.86	1751020	20.0
Heneicosane	14.64	6.3	ng	381176	6	15.26	1210570	20.0
Tricosane	14.96	8.0	ng	486131	6	15.26	1210570	20.0
Heptadecane, 2,6,...	15.32	6.1	ng	366723	6	15.26	1210570	20.0
Tetradecane, 2,6,...	15.72	6.2	ng	375441	6	15.26	1210570	20.0
Docosane	16.19	3.9	ng	237881	6	15.26	1210570	20.0