LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112742.D
Acq On : 28 Feb 2019 2:11
Operator : JU/SJ
Sample : K1596-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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	4.940	481	485	491	rBV	52498	67113	1.58%	0.145%
2	5.351	550	555	558	rBV	4058191	4042354	94.99%	8.716%
3	6.375	723	729	732	rBV	4311868	4255556	100.00%	9.176%
4	6.510	747	752	755	rBV	4621379	4236758	99.56%	9.136%
5	6.740	788	791	795	rBV	1467875	1229095	28.88%	2.650%
6	6.898	814	818	821	rBV	3730438	3034967	71.32%	6.544%
7	7.298	881	886	889	rBV	2840673	2543584	59.77%	5.485%
8	8.022	1005	1009	1012	rBV	1833527	1473459	34.62%	3.177%
9	9.098	1188	1192	1195	rBV	4303443	3490015	82.01%	7.525%
10	9.192	1205	1208	1211	rVB2	58034	48258	1.13%	0.104%
11	9.434	1244	1249	1251	rBV	38119	44265	1.04%	0.095%
12	9.486	1255	1258	1261	rBV	284441	222044	5.22%	0.479%
13	9.628	1279	1282	1285	rBV	61229	52755	1.24%	0.114%
14	9.769	1301	1306	1310	rBV2	1691684	1486777	34.94%	3.206%
15	9.804	1310	1312	1315	rVB	122209	96259	2.26%	0.208%
16	9.975	1338	1341	1345	rVB	90079	81370	1.91%	0.175%
17	10.316	1396	1399	1402	rBV	108463	94384	2.22%	0.204%
18	10.551	1435	1439	1443	rBV	2789739	2553940	60.01%	5.507%
19	10.686	1459	1462	1470	rVB5	56373	81123	1.91%	0.175%
20	10.922	1499	1502	1505	rBV2	60469	62777	1.48%	0.135%
21	11.051	1521	1524	1529	rVB	61278	67916	1.60%	0.146%
22	11.116	1529	1535	1536	rBV4	45155	75716	1.78%	0.163%
23	11.139	1536	1539	1542	rVB2	67382	78961	1.86%	0.170%
24	11.245	1554	1557	1559	rBV	1737185	1550544	36.44%	3.343%
25	11.269	1559	1561	1564	rVB	1096824	863068	20.28%	1.861%
26	11.322	1564	1570	1573	rBV	285386	270833	6.36%	0.584%
27	11.469	1590	1595	1599	rBV2	87508	106563	2.50%	0.230%
28	11.563	1606	1611	1612	rBV3	33647	45516	1.07%	0.098%
29	11.727	1636	1639	1640	rBV	46072	46099	1.08%	0.099%
30	11.745	1640	1642	1645	rVV	124079	120982	2.84%	0.261%
31	11.786	1645	1649	1652	rVV2	588508	683945	16.07%	1.475%
32	11.822	1652	1655	1658	rVV2	129154	154073	3.62%	0.332%
33	11.857	1658	1661	1663	rVV	215753	220716	5.19%	0.476%
34	11.880	1663	1665	1668	rVB	110644	86861	2.04%	0.187%

LSC Area Percent Report

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Sample : K1596-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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	12.045	1690	1693	1694	rBV	97033	92081	2.16%	0.199%
36	12.298	1732	1736	1739	rBV	165164	166404	3.91%	0.359%
37	12.333	1739	1742	1744	rVV3	71519	76668	1.80%	0.165%
38	12.374	1747	1749	1755	rVB3	54661	66246	1.56%	0.143%
39	12.451	1759	1762	1766	rBV	1263210	1141037	26.81%	2.460%
40	12.569	1780	1782	1786	rBV2	153634	163947	3.85%	0.354%
41	12.680	1796	1801	1804	rBV	1211041	1188499	27.93%	2.563%
42	12.704	1804	1805	1807	rVB	100507	69219	1.63%	0.149%
43	12.798	1819	1821	1823	rBV	79069	75211	1.77%	0.162%
44	12.833	1823	1827	1830	rVB	3509700	3415235	80.25%	7.364%
45	12.992	1851	1854	1855	rBV2	67009	81930	1.93%	0.177%
46	13.010	1855	1857	1860	rVB	167316	140657	3.31%	0.303%
47	13.074	1866	1868	1871	rVB	149689	125009	2.94%	0.270%
48	13.110	1871	1874	1877	rBV	141145	143717	3.38%	0.310%
49	13.233	1893	1895	1899	rBV2	72581	68430	1.61%	0.148%
50	13.310	1905	1908	1916	rVB3	131233	181288	4.26%	0.391%
51	13.733	1977	1980	1988	rVB	912070	862085	20.26%	1.859%
52	13.874	1999	2004	2006	rBV2	1679987	1912456	44.94%	4.124%
53	13.898	2006	2008	2010	rVB	449100	326054	7.66%	0.703%
54	14.063	2033	2036	2038	rBV	147360	142496	3.35%	0.307%
55	14.368	2085	2088	2092	rBV2	180597	199597	4.69%	0.430%
56	14.516	2111	2113	2117	rVB	221985	198469	4.66%	0.428%
57	14.663	2136	2138	2145	rVB3	174338	202129	4.75%	0.436%
58	14.880	2173	2175	2178	rBV	215598	287754	6.76%	0.620%
59	14.980	2190	2192	2199	rVB	262557	297405	6.99%	0.641%
60	15.168	2221	2224	2228	rBV	170237	188610	4.43%	0.407%
61	15.221	2231	2233	2236	rVB	215060	184943	4.35%	0.399%
62	15.280	2240	2243	2247	rVB	667191	810360	19.04%	1.747%

Sum of corrected areas: 46376582

LSC Report - Integrated Chromatogram

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Data File : BF112742.D
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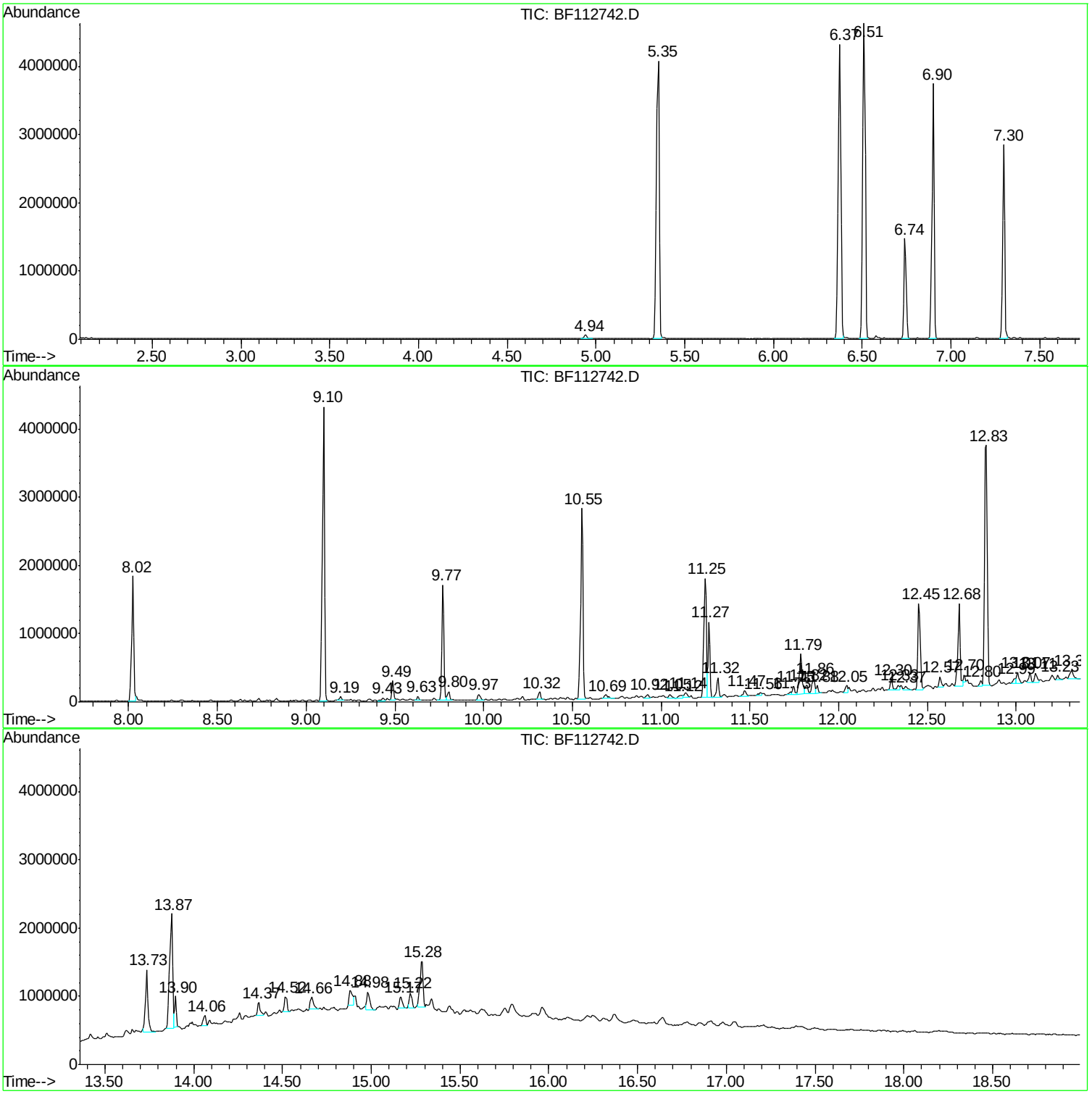
Sample : K1596-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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\BF022719\
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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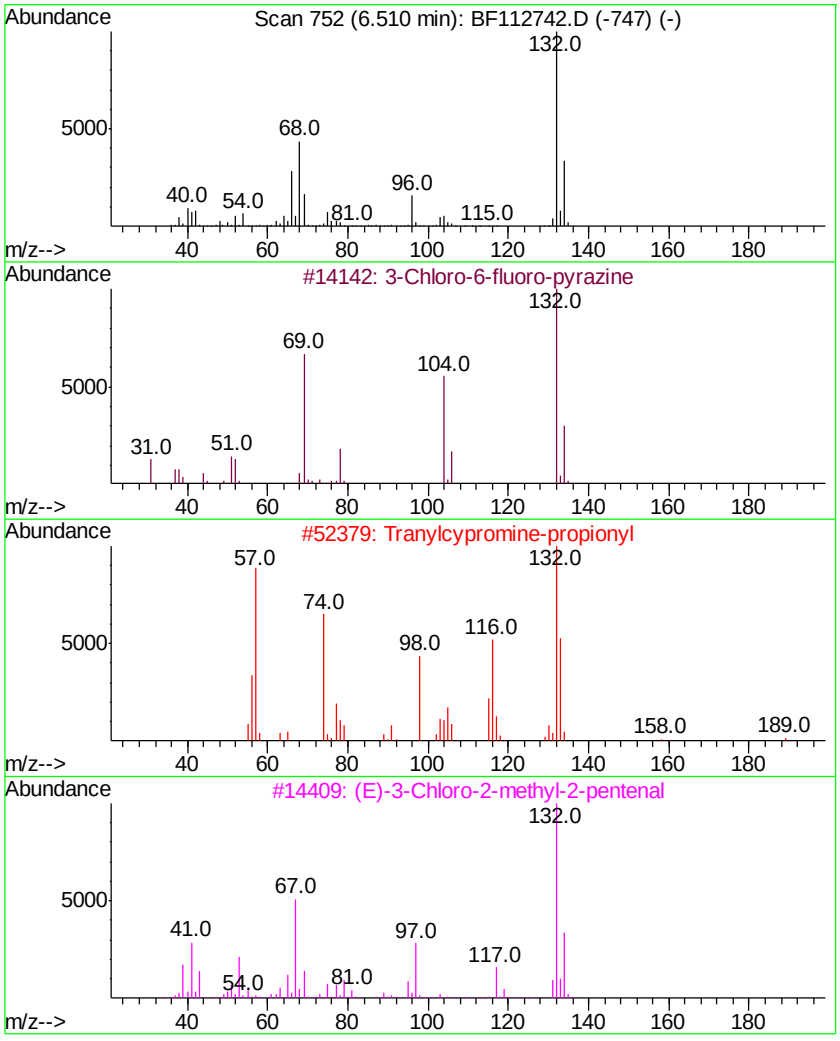
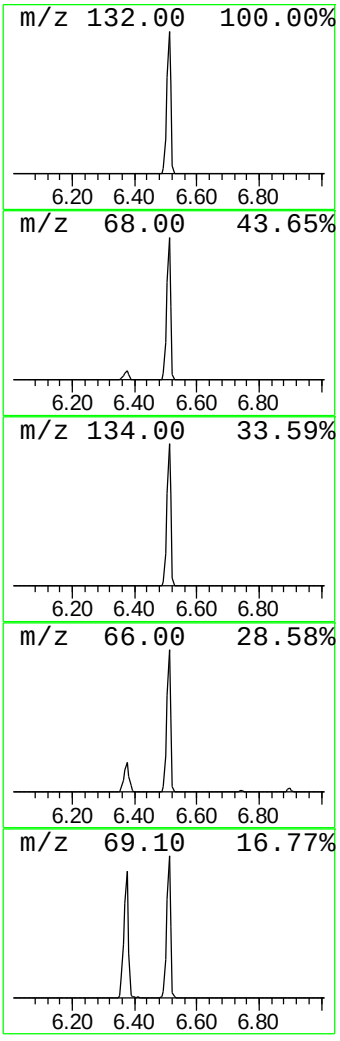
Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	68.94 ng	4236760	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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

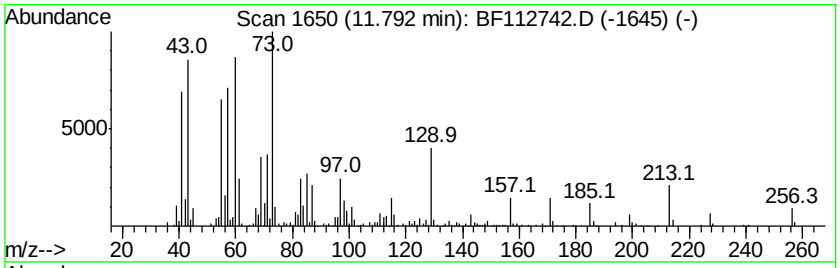
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

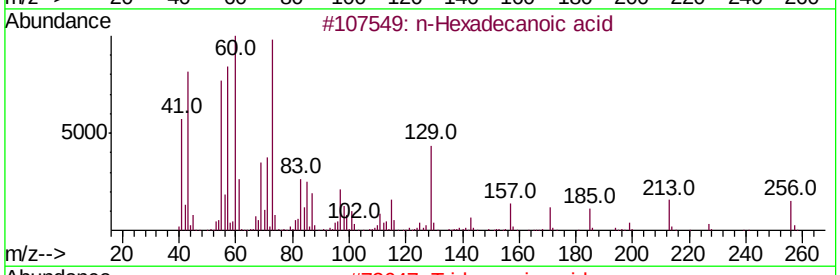
****

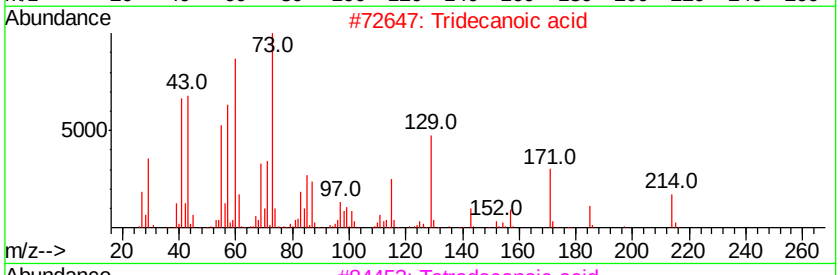
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

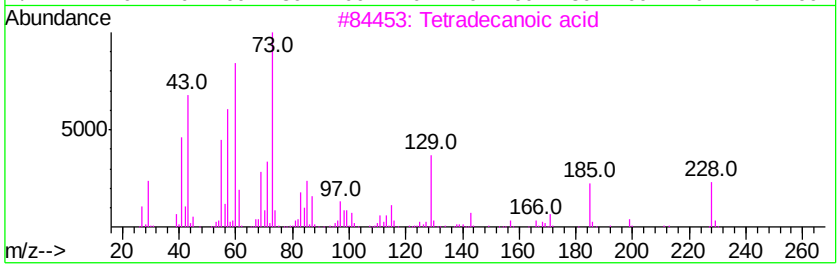
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	8.82 ng	683945	Phenanthrene-d10	11.25

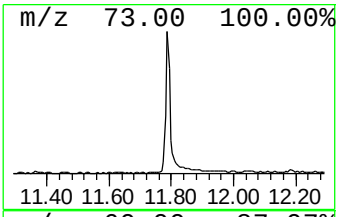
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64

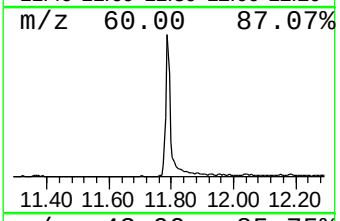


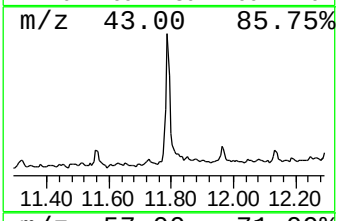


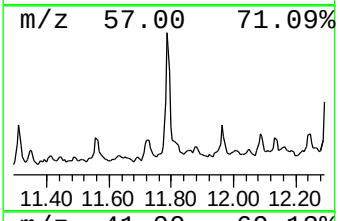


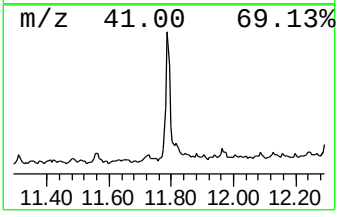












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Instrument : BNA_F
ClientSampleId : COMP-13

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

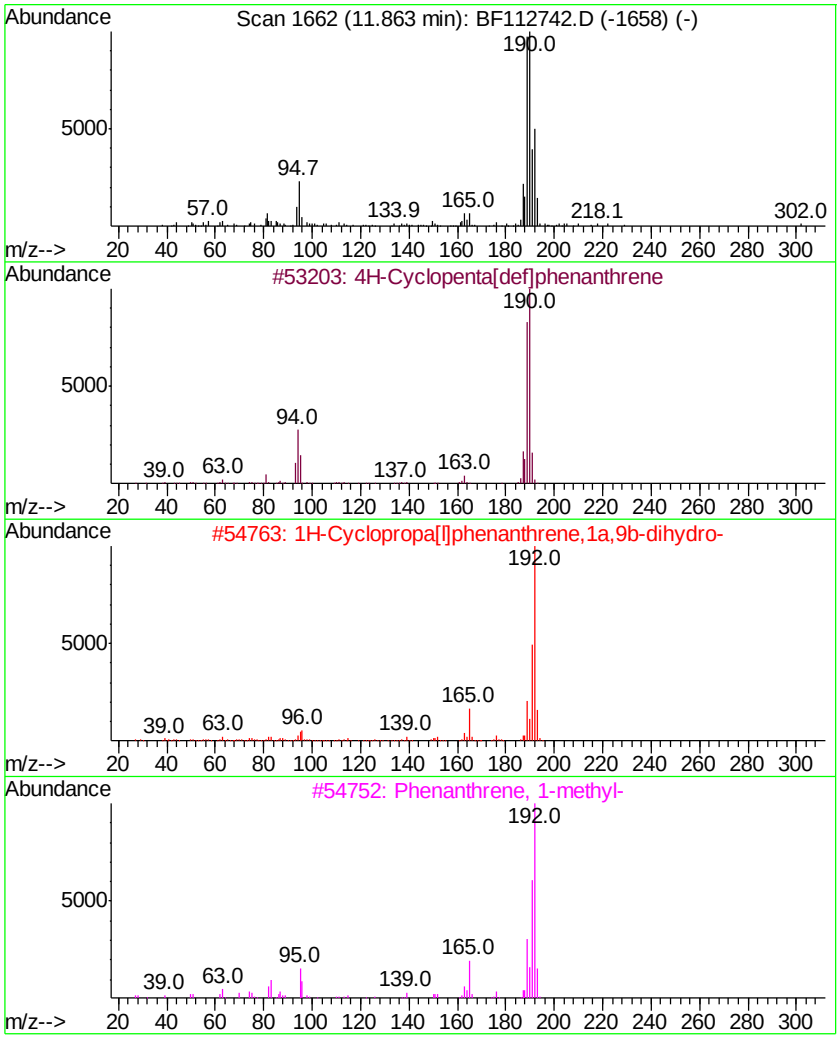
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

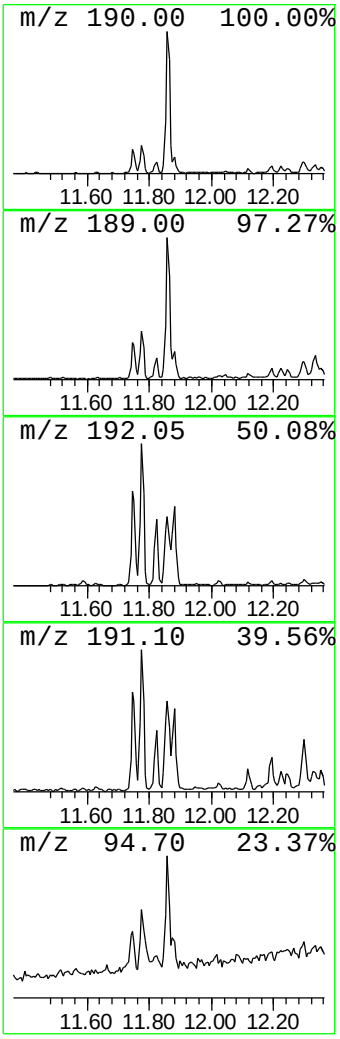
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.85 ng	220716	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	38
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30





Library Search Compound Report

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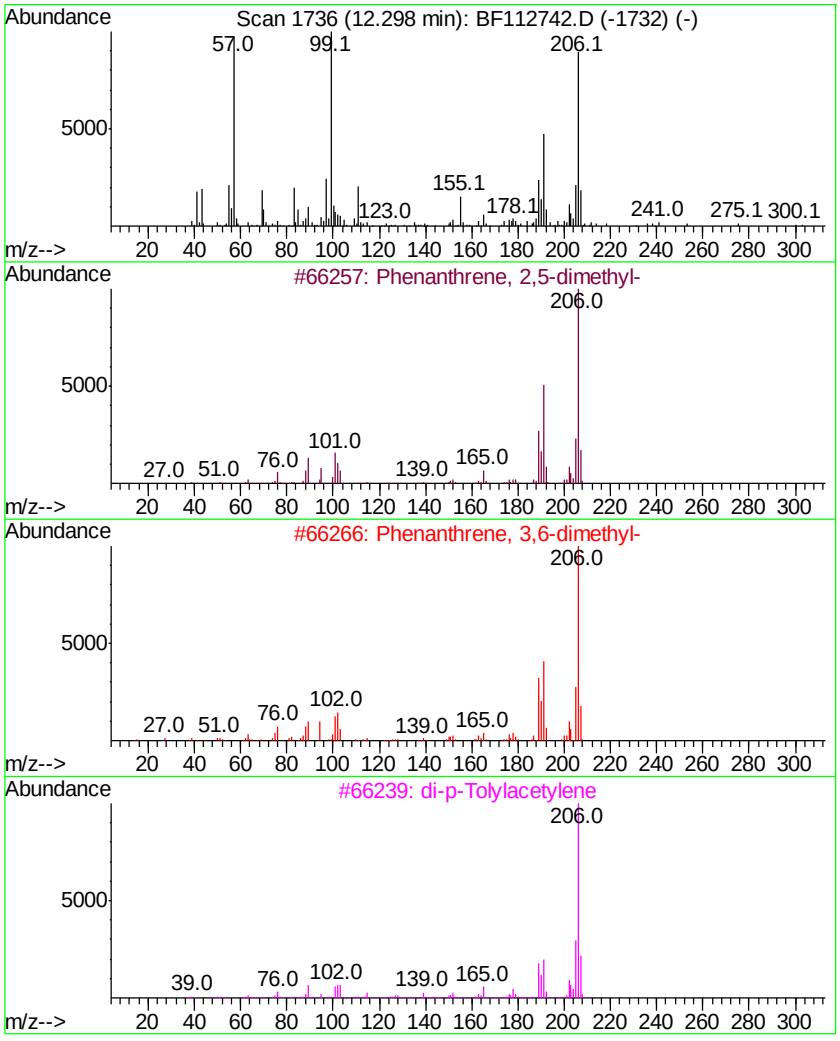
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

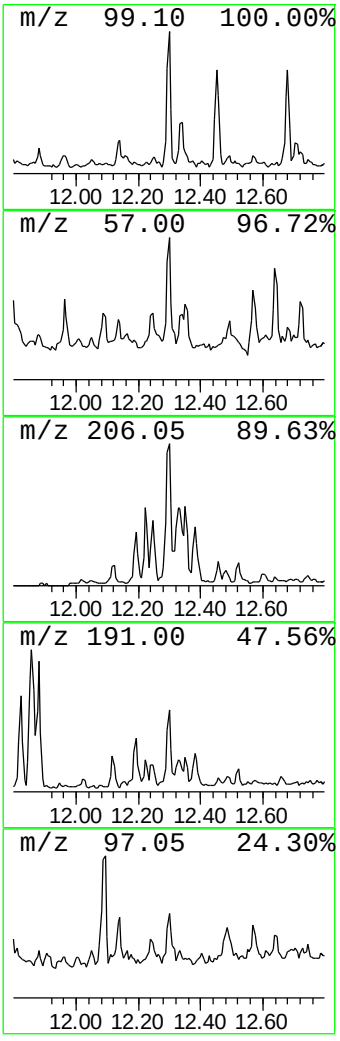
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.15 ng	166404	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	70
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	64
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	59
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	55
5	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	50





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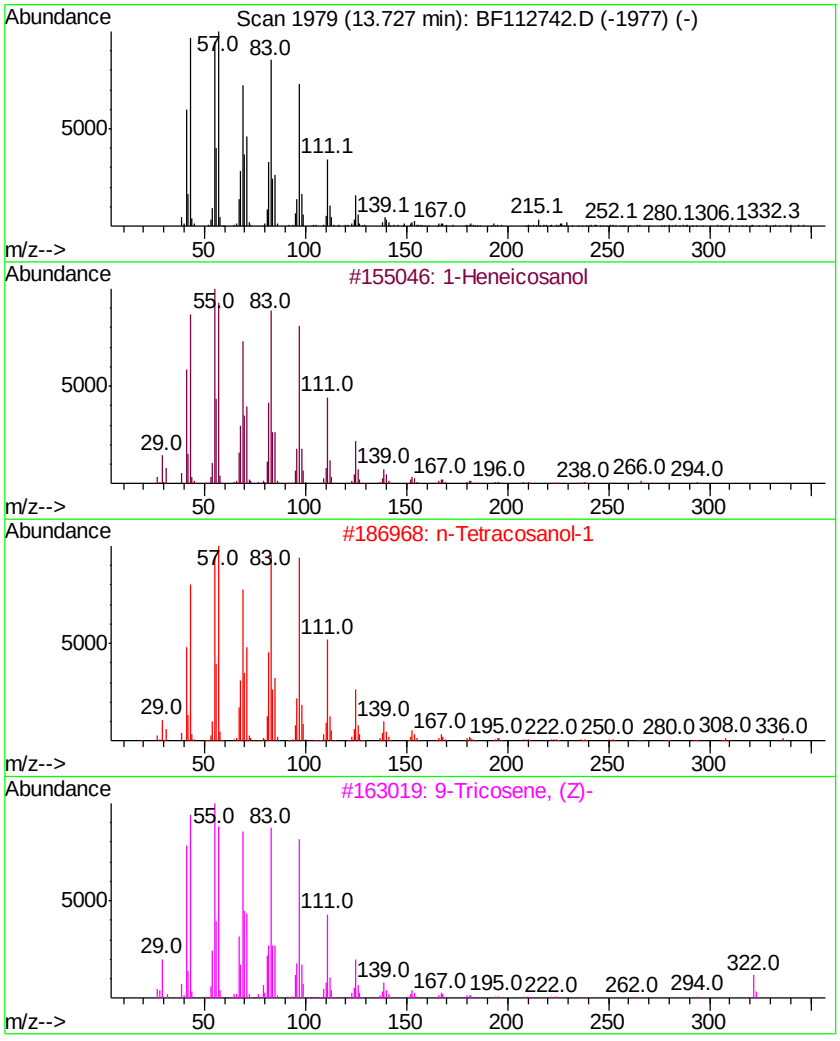
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

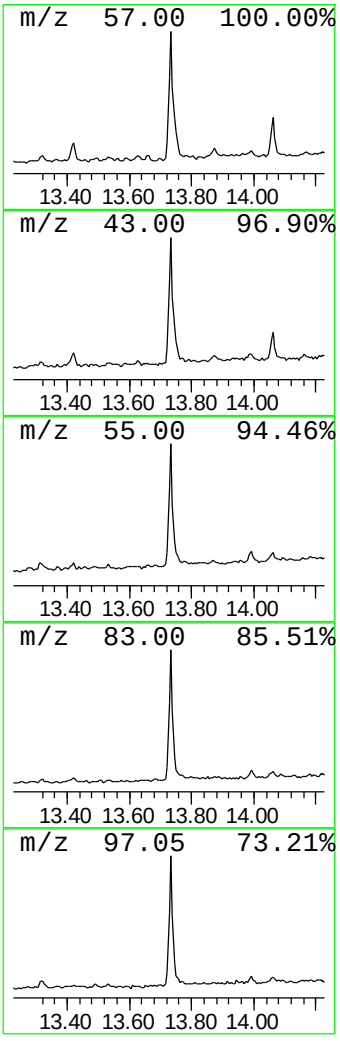
****

Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	9.02 ng	862085	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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Data File : BF112742.D
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Operator : JU/SJ
Sample : K1596-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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

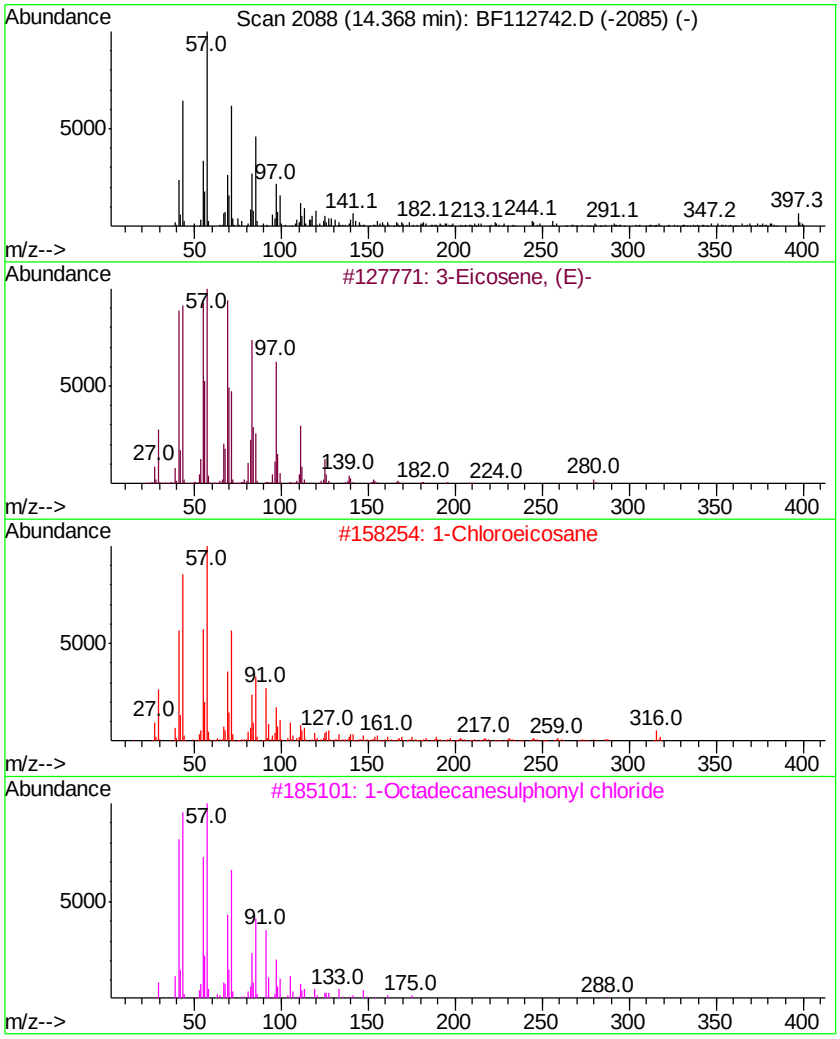
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

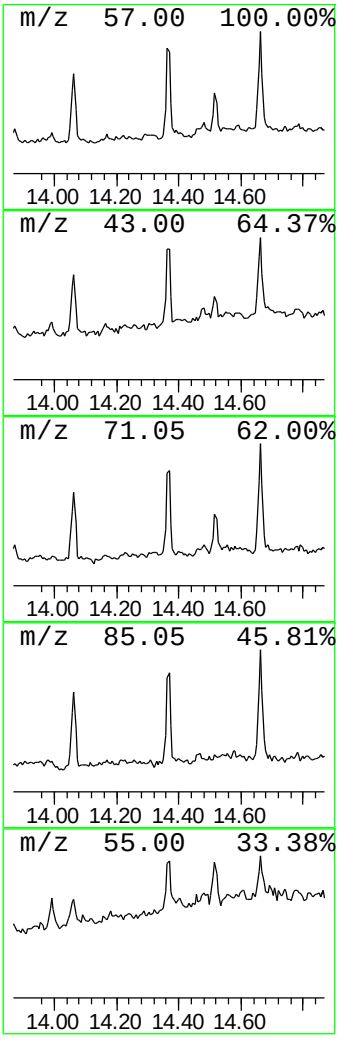
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.09 ng	199597	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	1-Chloroeicosane	316	C20H41Cl	042217-02-7	94
3	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
4	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91





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Data File : BF112742.D
Acq On : 28 Feb 2019 2:11
Operator : JU/SJ
Sample : K1596-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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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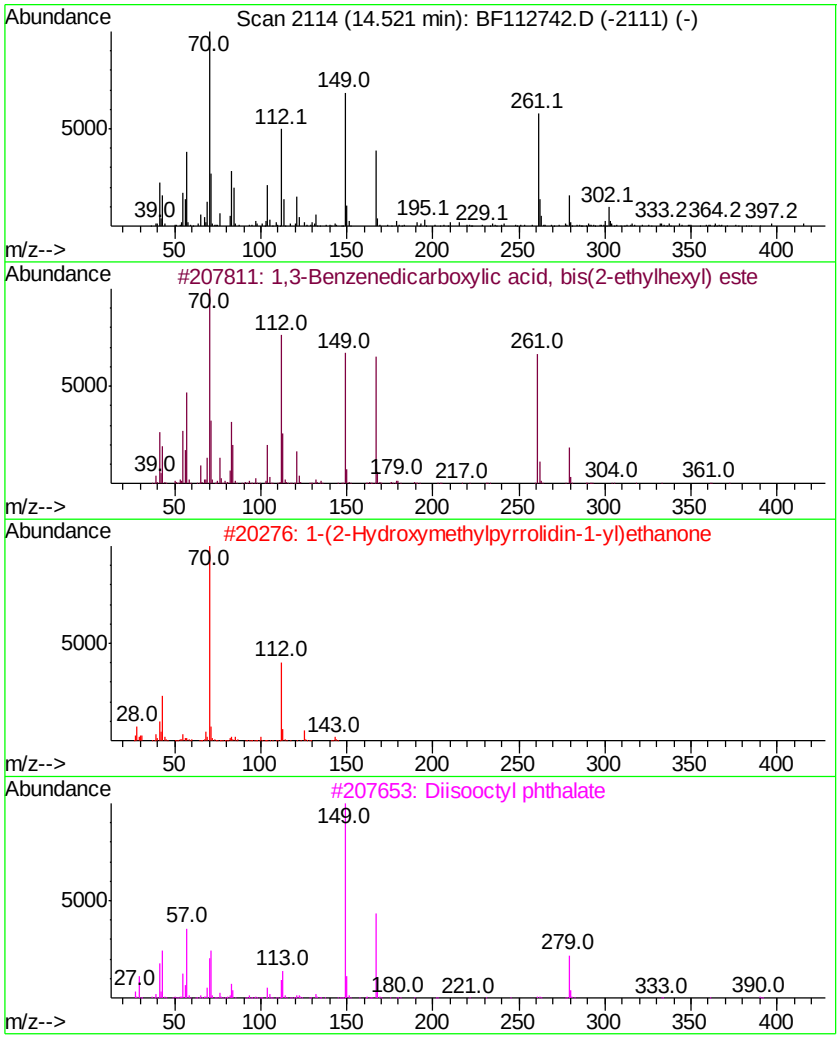
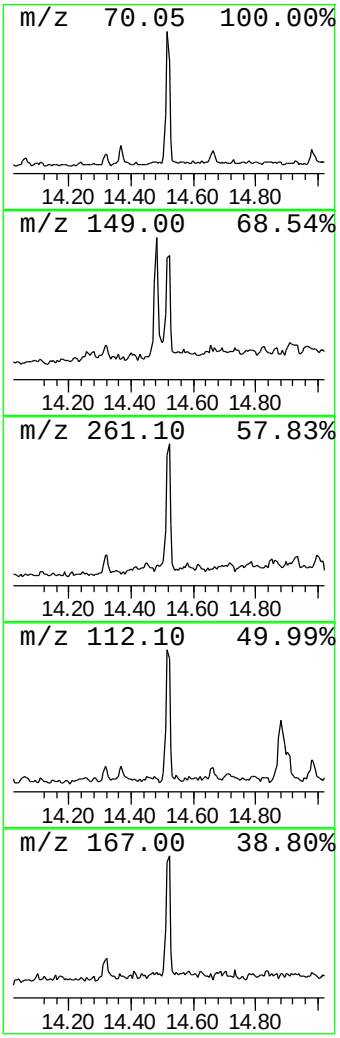
Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.08 ng	198469	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
2	1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	30
3	Diisooctyl phthalate	390	C24H38O4	000131-20-4	14
4	Undecane, 3-methylene-	168	C12H24	071138-64-2	14
5	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	14





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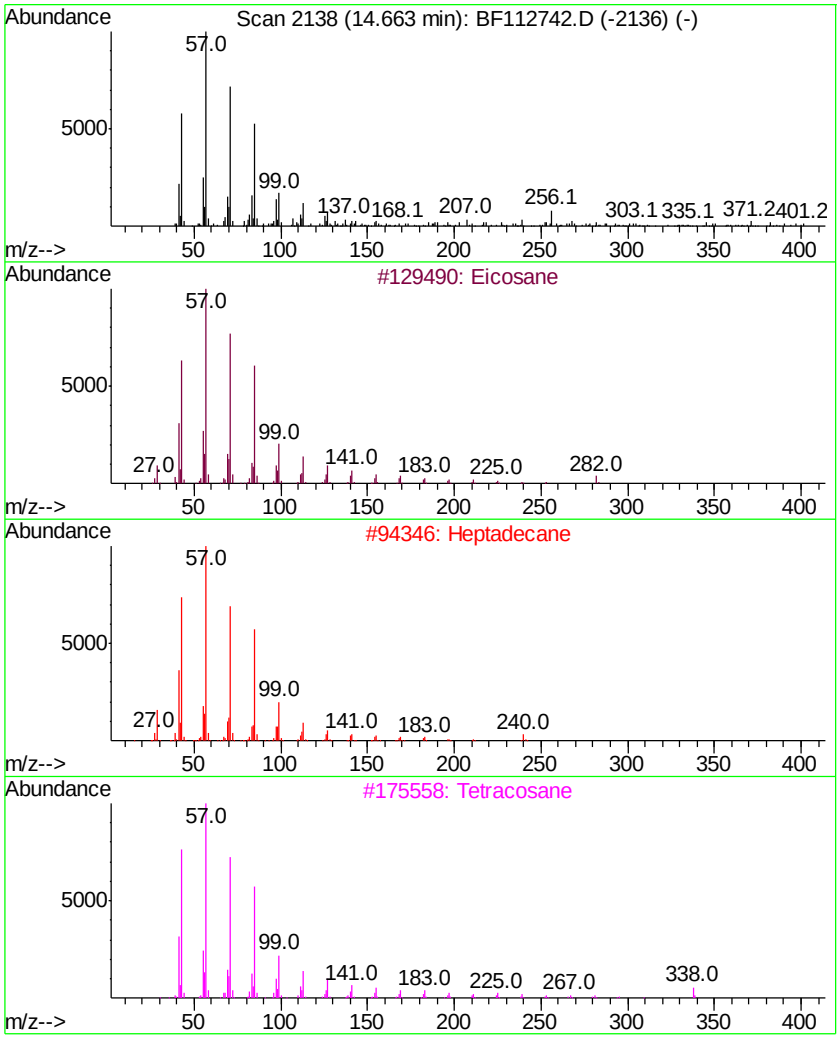
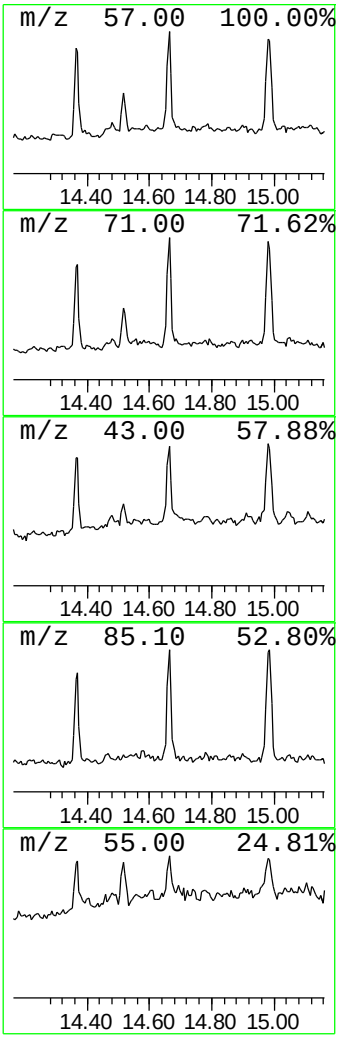
Peak Number 9 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	4.99 ng	202129	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Heptadecane	240	C17H36	000629-78-7	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Octacosane	394	C28H58	000630-02-4	76
5	Tetradecane	198	C14H30	000629-59-4	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112742.D
Acq On : 28 Feb 2019 2:11
Operator : JU/SJ
Sample : K1596-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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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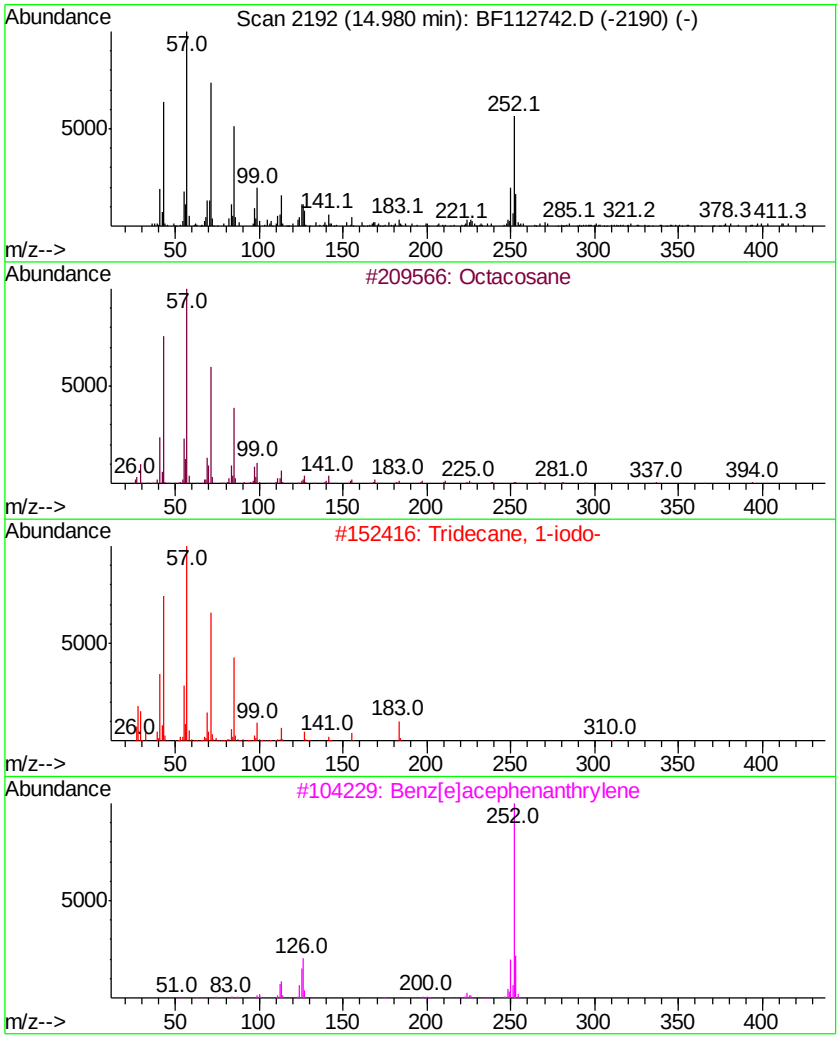
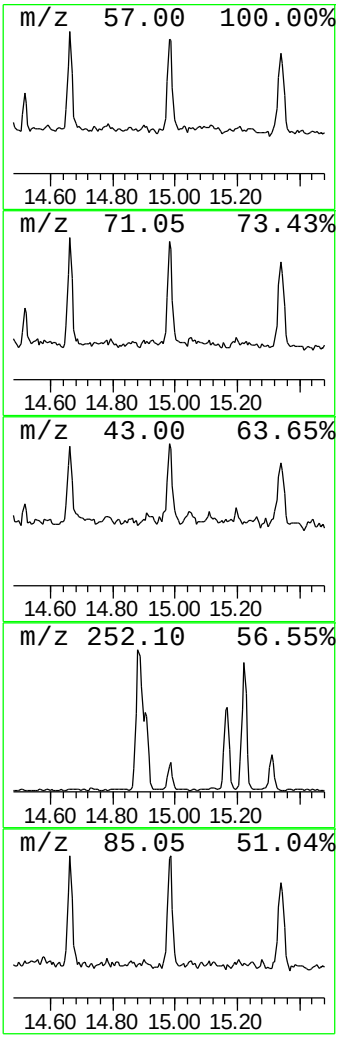
Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	7.34 ng	297405	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	70
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	64
4	Heneicosane	296	C21H44	000629-94-7	64
5	Octadecane	254	C18H38	000593-45-3	60





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Acq On : 28 Feb 2019 2:11
Operator : JU/SJ
Sample : K1596-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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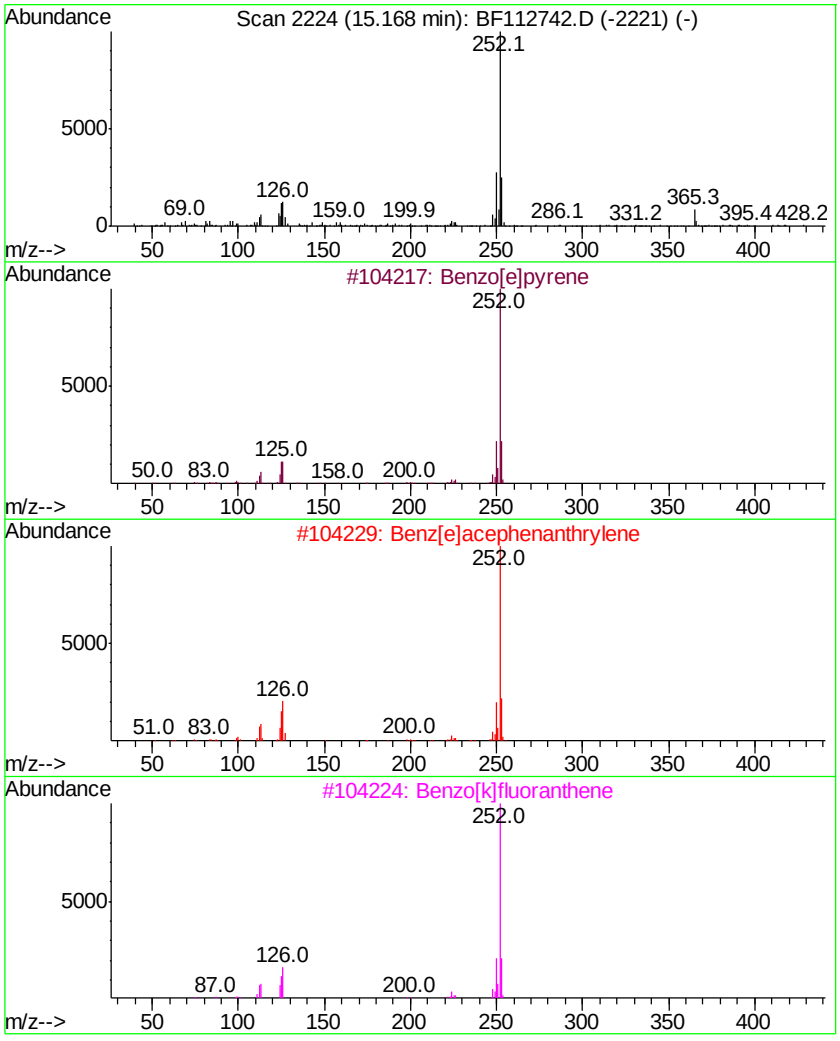
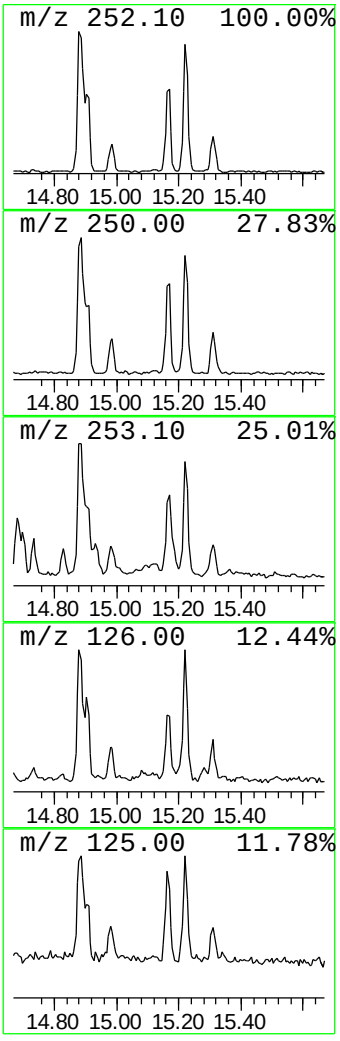
Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	4.65 ng	188610	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	97
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Perylene	252	C20H12	000198-55-0	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022719\
Data File : BF112742.D
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Operator : JU/SJ
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-13

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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
unknown6.51	6.51	68.9	ng	4236760	1	6.74	1229100	20.0
n-Hexadecanoic acid	11.79	8.8	ng	683945	4	11.25	1550540	20.0
4H-Cyclopenta[def...	11.86	2.9	ng	220716	4	11.25	1550540	20.0
Phenanthrene, 2,5...	12.30	2.1	ng	166404	4	11.25	1550540	20.0
1-Heneicosanol	13.73	9.0	ng	862085	5	13.87	1912460	20.0
3-Eicosene, (E)-	14.37	2.1	ng	199597	5	13.87	1912460	20.0
1,3-Benzenedicarb...	14.52	2.1	ng	198469	5	13.87	1912460	20.0
Eicosane	14.66	5.0	ng	202129	6	15.28	810360	20.0
Octacosane	14.98	7.3	ng	297405	6	15.28	810360	20.0
Benzo[e]pyrene	15.17	4.7	ng	188610	6	15.28	810360	20.0