LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116407.D
Acq On : 20 Aug 2019 00:11
Operator : HP/JU
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

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-BF073019.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	5.434	566	569	605	rBV	2439873	2802876	76.86%	7.773%
2	6.451	739	742	760	rBV	2555437	3007890	82.49%	8.342%
3	6.581	760	764	772	rVB	3125725	2955162	81.04%	8.196%
4	6.804	799	802	812	rVB	661949	596451	16.36%	1.654%
5	6.957	825	828	844	rBV	2478846	2382830	65.35%	6.608%
6	7.369	894	898	919	rBV	2040449	1957137	53.67%	5.428%
7	8.081	1016	1019	1038	rVB	788717	788240	21.62%	2.186%
8	9.157	1198	1202	1205	rBV	3640982	3334247	91.44%	9.247%
9	9.551	1265	1269	1279	rVB	483417	410634	11.26%	1.139%
10	9.834	1313	1317	1321	rBV	1134520	937073	25.70%	2.599%
11	10.628	1448	1452	1462	rBV	2389955	2324346	63.74%	6.446%
12	11.322	1566	1570	1572	rBV	1206600	1011555	27.74%	2.805%
13	11.345	1572	1574	1579	rVB	595469	508527	13.95%	1.410%
14	11.404	1582	1584	1587	rVB	79149	65744	1.80%	0.182%
15	11.569	1609	1612	1616	rBV2	44977	43539	1.19%	0.121%
16	11.845	1656	1659	1667	rVB2	412074	484437	13.28%	1.343%
17	11.939	1672	1675	1677	rBV	89720	92164	2.53%	0.256%
18	11.963	1677	1679	1684	rVB	50957	47941	1.31%	0.133%
19	12.116	1703	1705	1711	rVB	63474	56683	1.55%	0.157%
20	12.169	1711	1714	1722	rVB2	48584	68990	1.89%	0.191%
21	12.374	1746	1749	1751	rBV	51215	45031	1.23%	0.125%
22	12.475	1761	1766	1773	rBV2	59492	77886	2.14%	0.216%
23	12.533	1773	1776	1782	rBV	1069612	1005677	27.58%	2.789%
24	12.633	1789	1793	1796	rBV3	52737	91596	2.51%	0.254%
25	12.692	1799	1803	1804	rBV	74195	72828	2.00%	0.202%
26	12.716	1804	1807	1809	rVV2	69724	91204	2.50%	0.253%
27	12.763	1809	1815	1822	rVB	1000973	1169786	32.08%	3.244%
28	12.904	1834	1839	1842	rVV	3506189	3646515	100.00%	10.113%
29	12.939	1843	1845	1849	rVB	42131	46172	1.27%	0.128%
30	12.992	1849	1854	1858	rVB2	48579	78865	2.16%	0.219%
31	13.074	1864	1868	1870	rBV2	43281	67437	1.85%	0.187%
32	13.098	1870	1872	1878	rVB3	60653	75202	2.06%	0.209%
33	13.204	1885	1890	1893	rBV2	71054	95498	2.62%	0.265%
34	13.327	1908	1911	1914	rBV2	42180	41748	1.14%	0.116%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-18

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-BF073019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.374	1914	1919	1922	rBV	463769	454546	12.47%	1.261%
36	13.616	1958	1960	1966	rVB	74578	72548	1.99%	0.201%
37	13.739	1975	1981	1984	rVB3	73486	131315	3.60%	0.364%
38	13.780	1984	1988	1994	rBV4	413315	579044	15.88%	1.606%
39	13.827	1994	1996	2001	rVB	90226	94635	2.60%	0.262%
40	13.921	2009	2012	2014	rBV	73705	65299	1.79%	0.181%
41	13.963	2014	2019	2022	rVV2	1010663	1270100	34.83%	3.522%
42	13.992	2022	2024	2031	rVB	332230	356159	9.77%	0.988%
43	14.357	2083	2086	2090	rBV	53873	53051	1.45%	0.147%
44	14.774	2154	2157	2162	rVB	236826	232502	6.38%	0.645%
45	15.004	2192	2196	2198	rBV	278016	371240	10.18%	1.030%
46	15.027	2198	2200	2206	rVB	201939	224314	6.15%	0.622%
47	15.110	2212	2214	2220	rVB	53590	66766	1.83%	0.185%
48	15.298	2243	2246	2250	rBV	153587	181188	4.97%	0.502%
49	15.363	2254	2257	2261	rBV	229234	288616	7.91%	0.800%
50	15.415	2263	2266	2271	rVV	533336	621149	17.03%	1.723%
51	15.868	2339	2343	2348	rBV5	39525	78809	2.16%	0.219%
52	16.886	2512	2516	2525	rVB	108371	196220	5.38%	0.544%
53	17.327	2587	2591	2606	rVB	98465	238615	6.54%	0.662%

Sum of corrected areas: 36058027

LSC Report - Integrated Chromatogram

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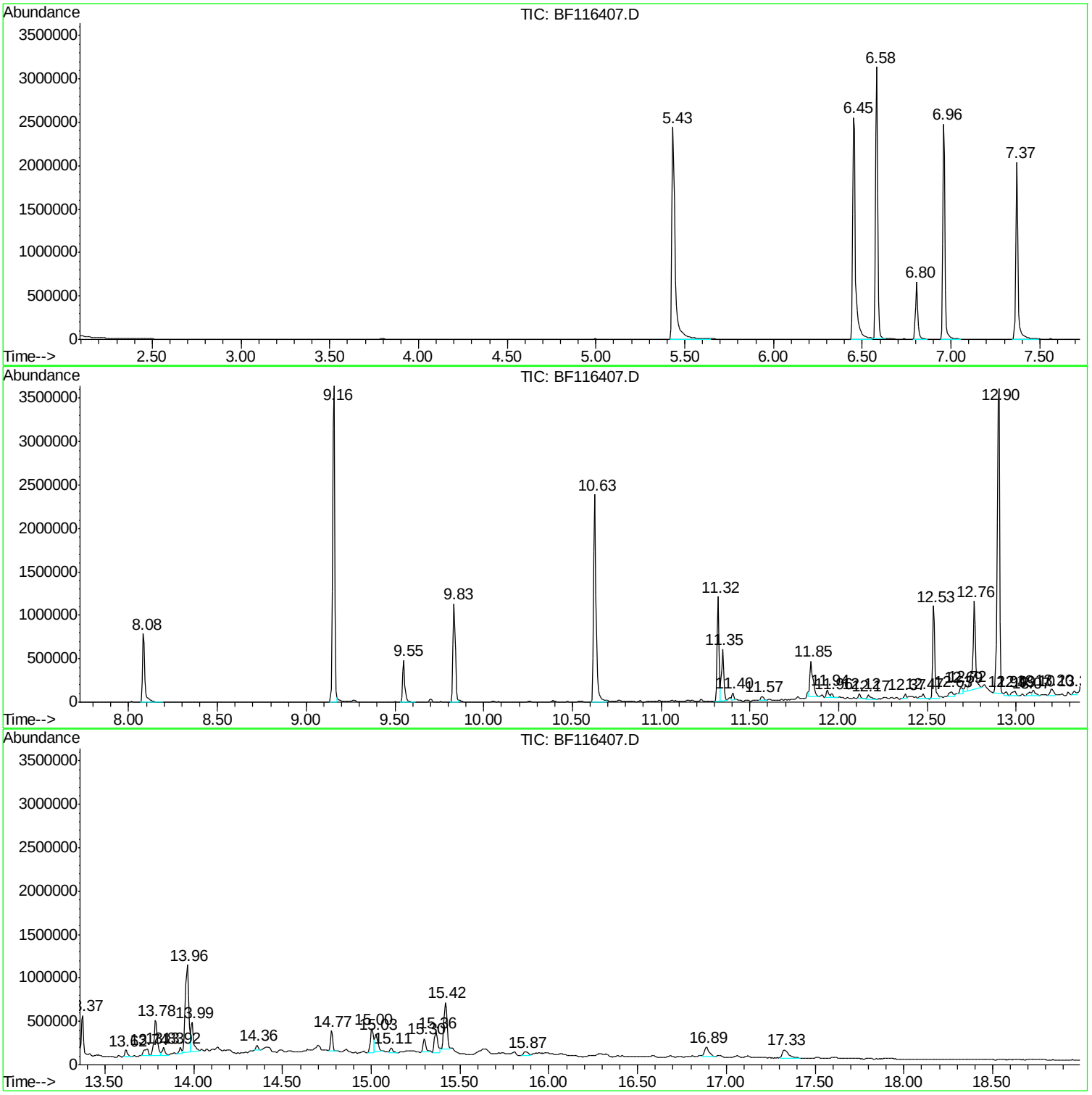
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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\BF081919\
Data File : BF116407.D
Acq On : 20 Aug 2019 00:11
Operator : HP/JU
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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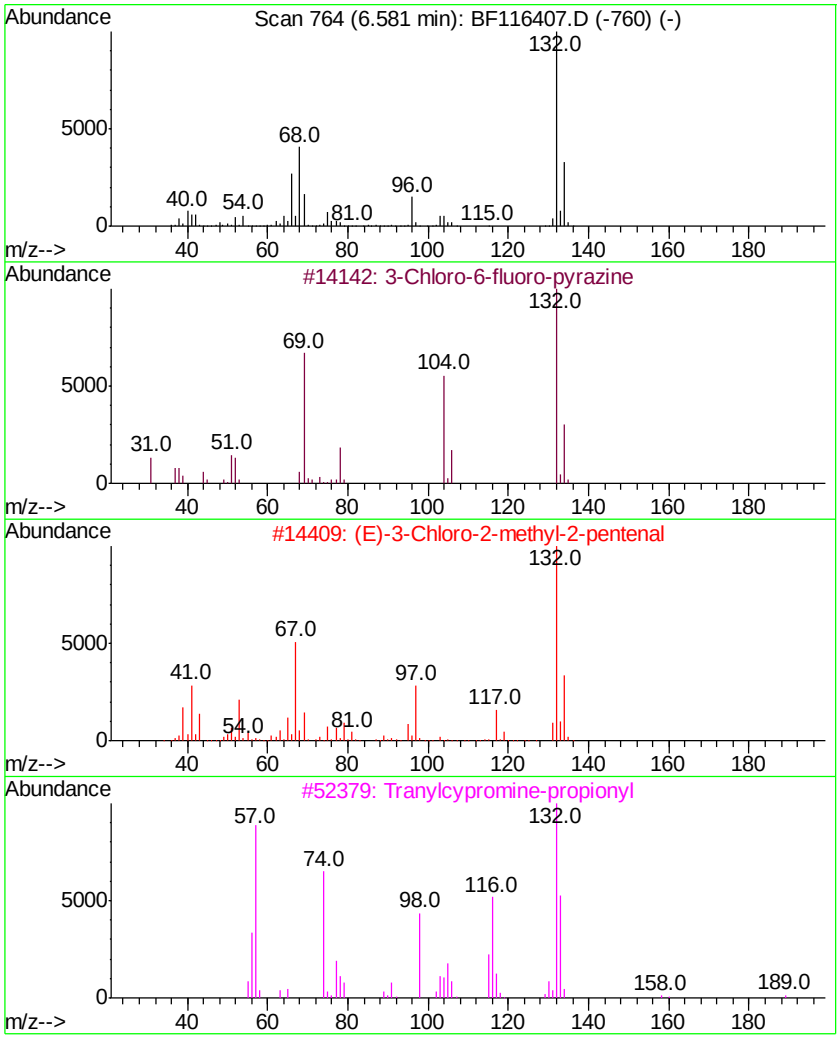
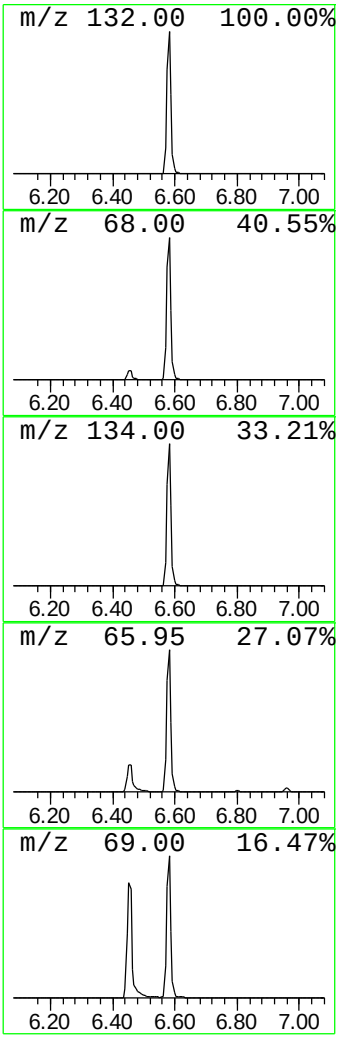
Peak Number 1 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	99.09 ng	2955160	1,4-Dichlorobenzene-d4	6.80

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	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Data File : BF116407.D
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Operator : HP/JU
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

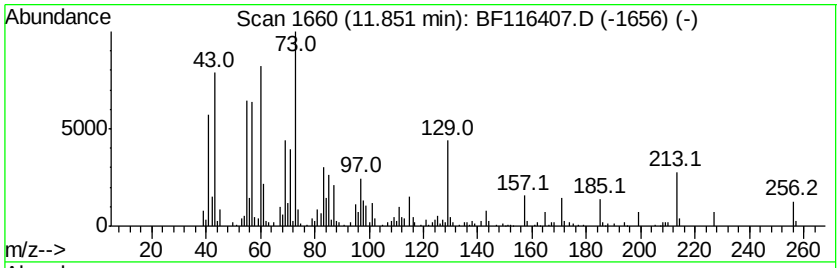
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

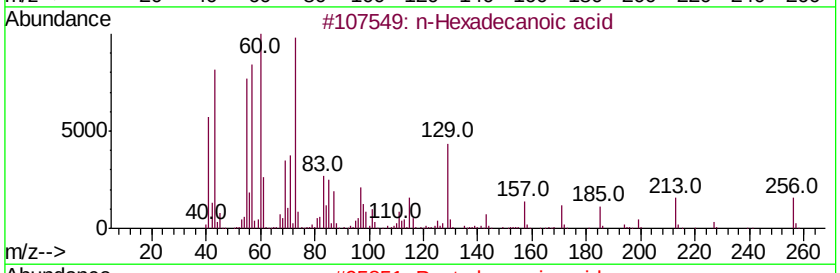
****

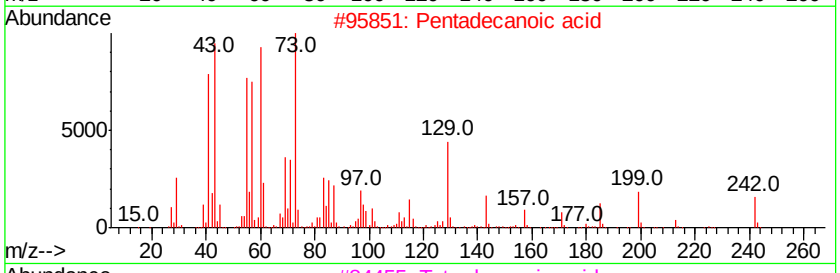
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

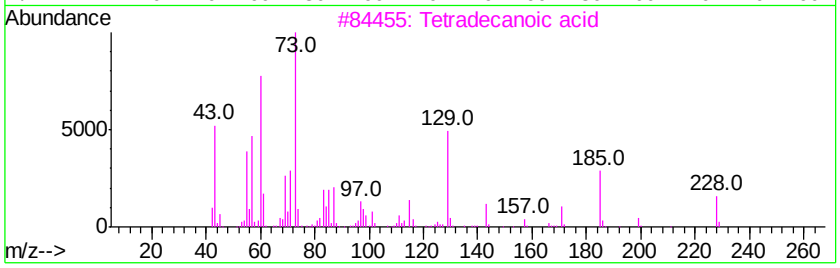
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	9.58 ng	484437	Phenanthrene-d10	11.32

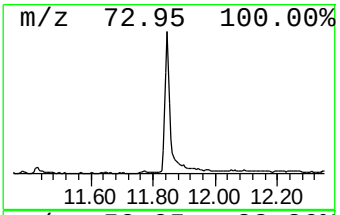
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62

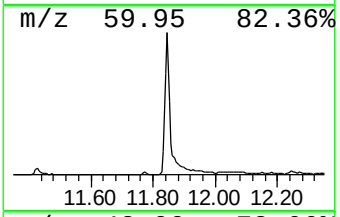


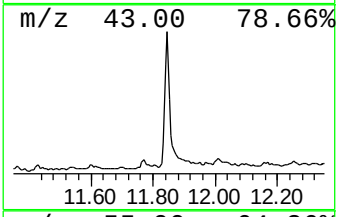


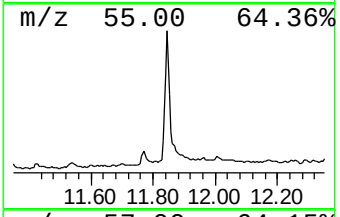


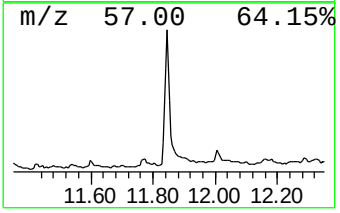












Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

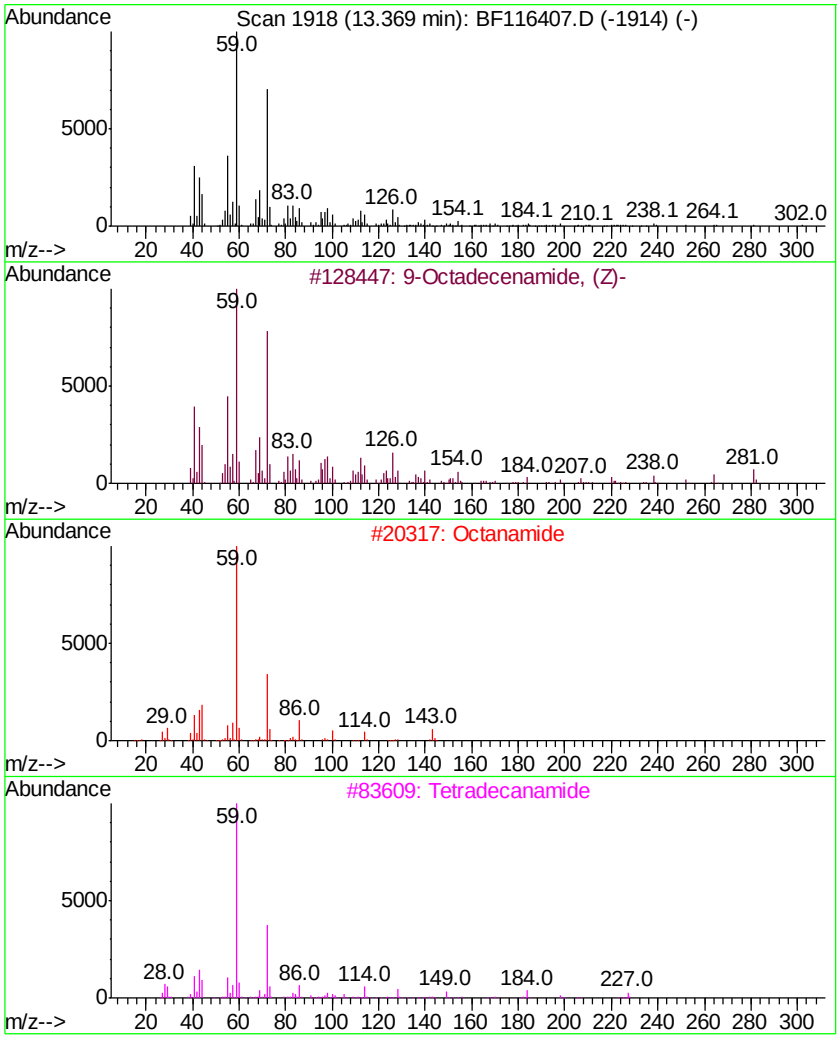
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

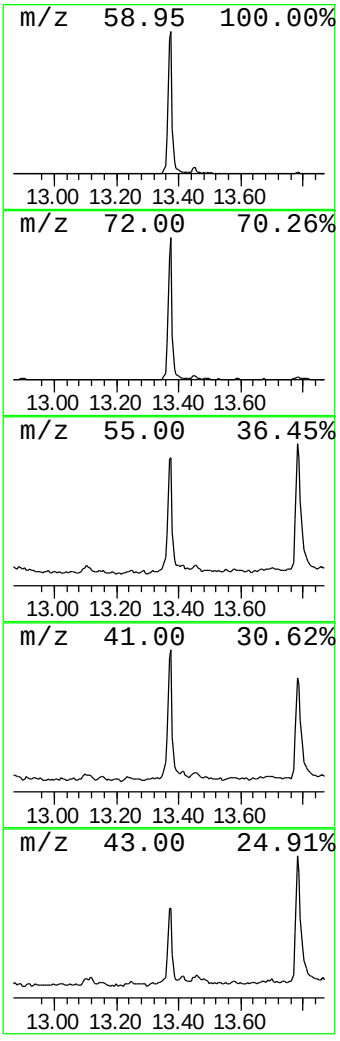
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	7.16 ng	454546	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Octanamide	143	C8H17NO	000629-01-6	47
3	Tetradecanamide	227	C14H29NO	000638-58-4	47
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	37
5	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	35





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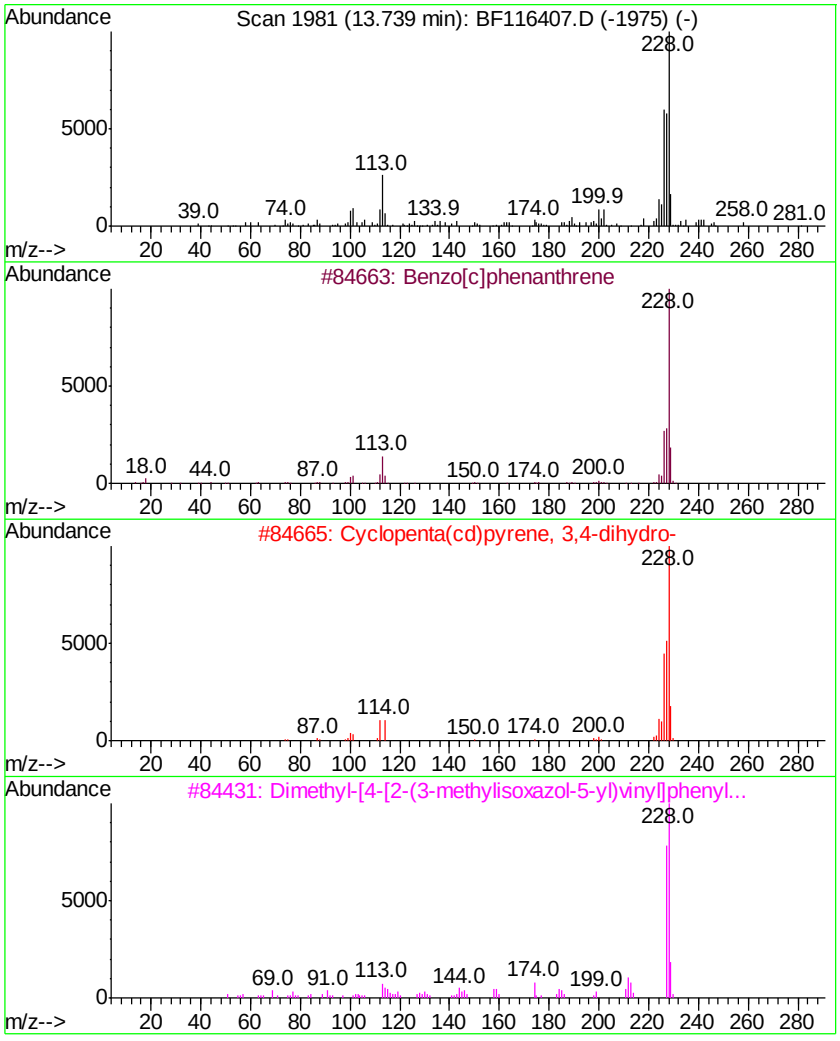
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

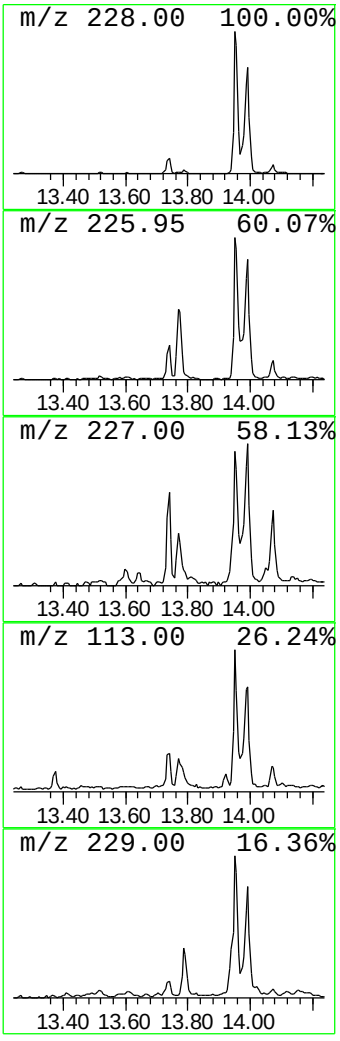
****

Peak Number 5 Benzo[c]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.07 ng	131315	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]phenanthrene	228	C18H12	000195-19-7	60
2	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	53
3	Dimethyl-[4-[2-(3-methylisoxazol...	228	C14H16N2O	1000306-39-6	47
4	Chrysene	228	C18H12	000218-01-9	46
5	Benz[a]anthracene	228	C18H12	000056-55-3	43





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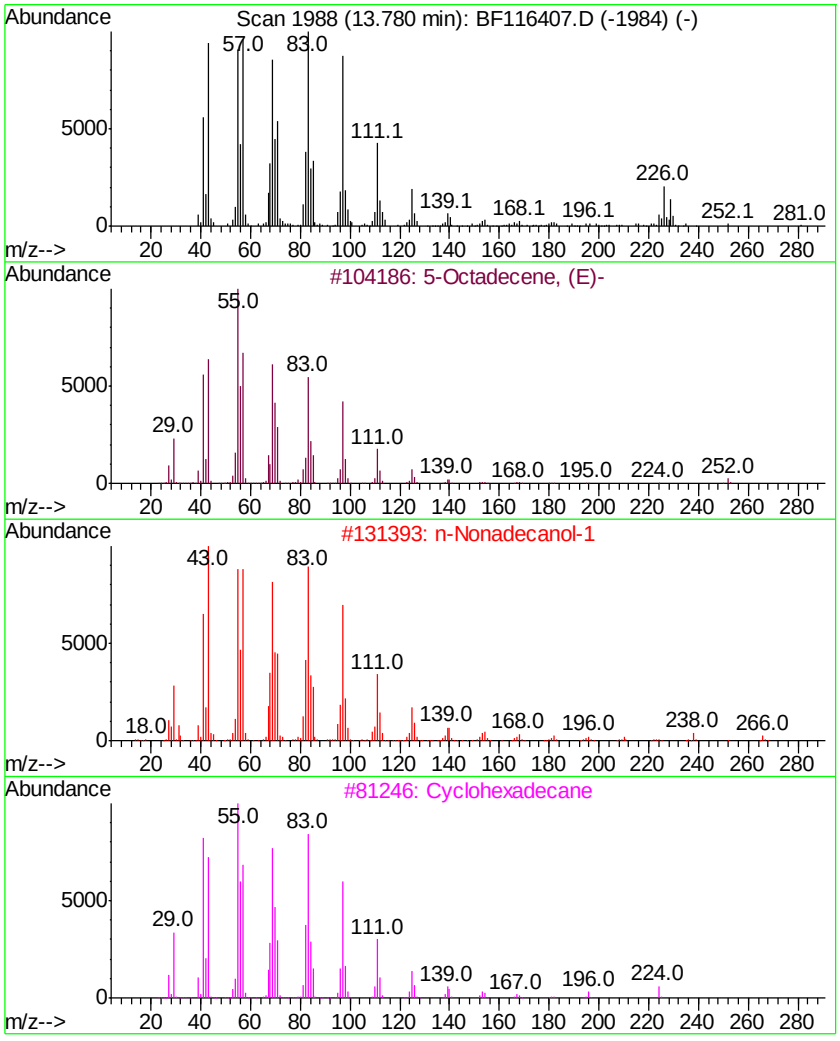
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

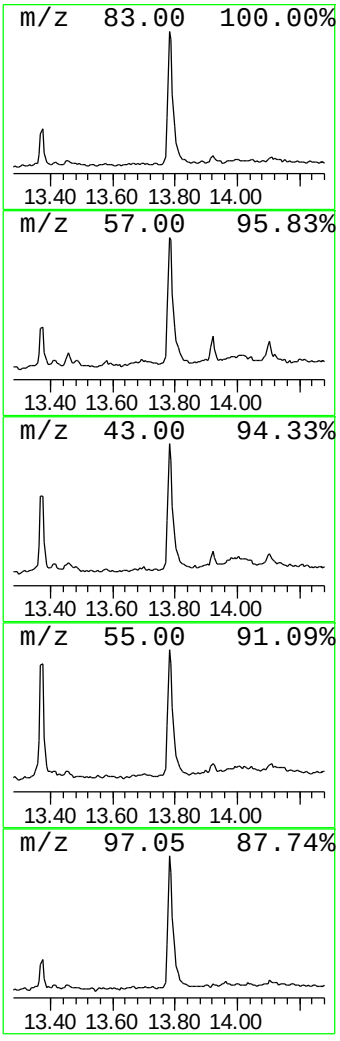
****

Peak Number 6 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	9.12 ng	579044	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Cyclohexadecane	224	C16H32	000295-65-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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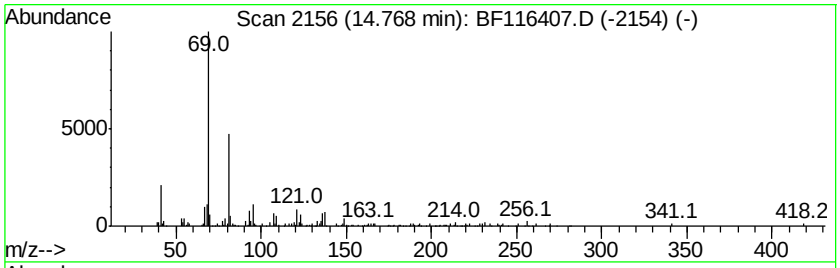
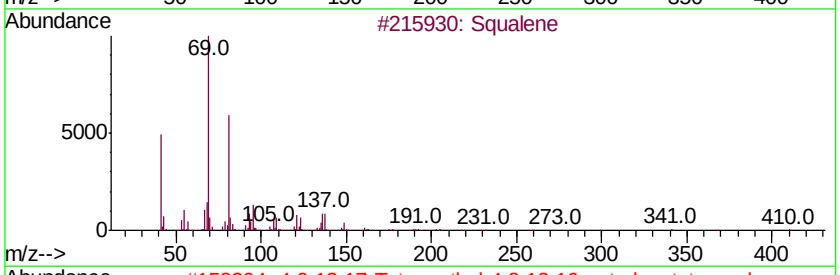
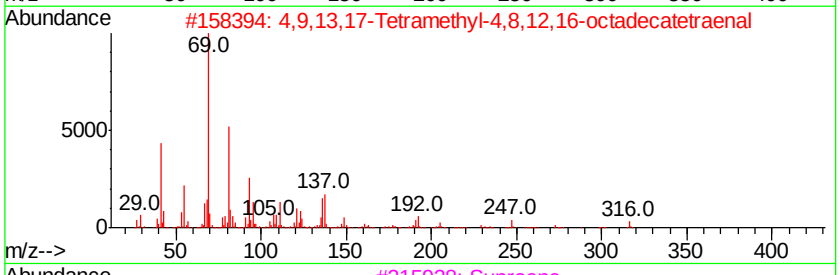
Peak Number 7 Squalene Concentration Rank 5

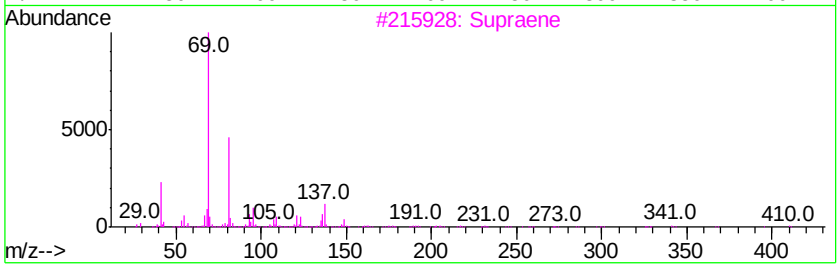
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	7.49 ng	232502	Perylene-d12	15.42

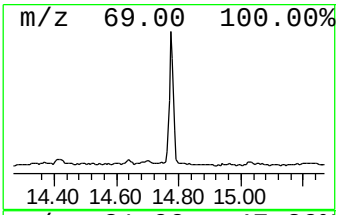
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3	Supraene	410	C30H50	007683-64-9	83
4	Farnesol isomer a	222	C15H26O	1000108-92-4	80
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72

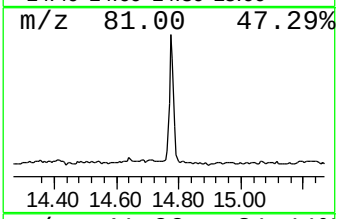


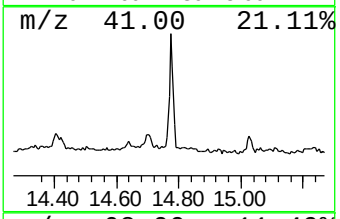


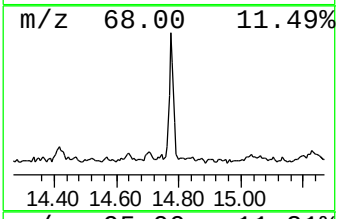


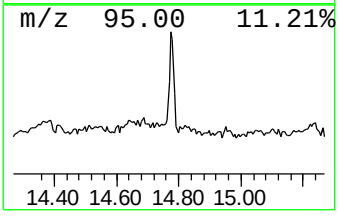












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116407.D
Acq On : 20 Aug 2019 00:11
Operator : HP/JU
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

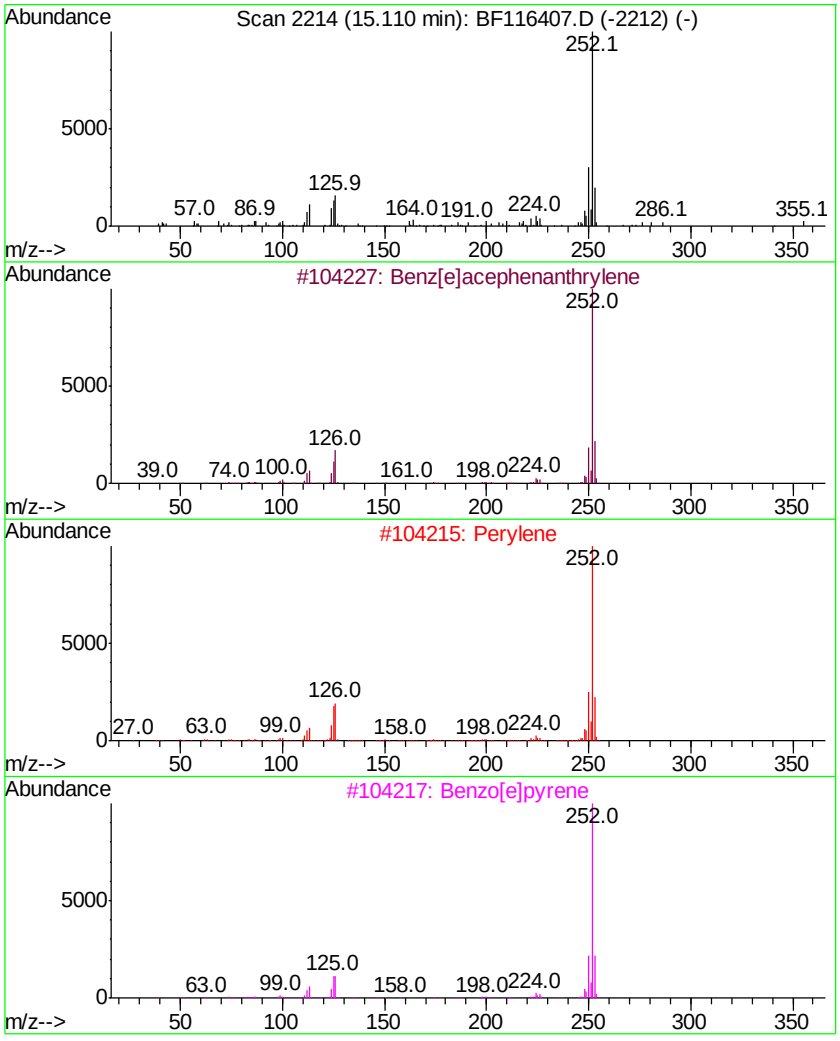
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

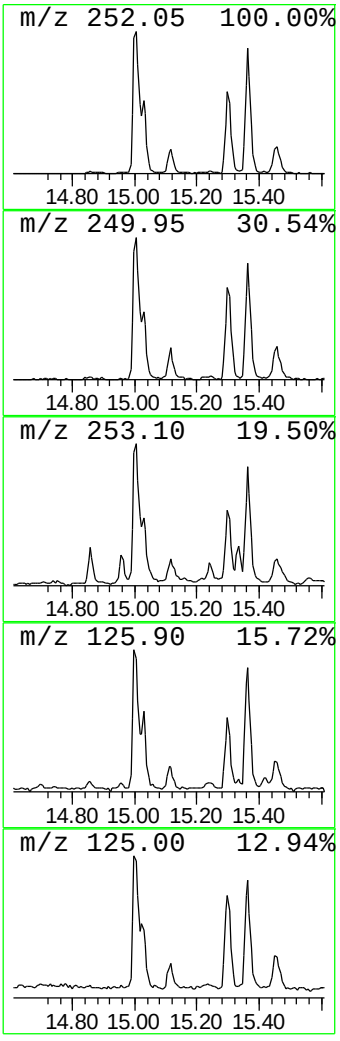
****

Peak Number 8 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.11	2.15 ng	66766	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
2	Perylene	252	C20H12	000198-55-0	94
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116407.D
Acq On : 20 Aug 2019 00:11
Operator : HP/JU
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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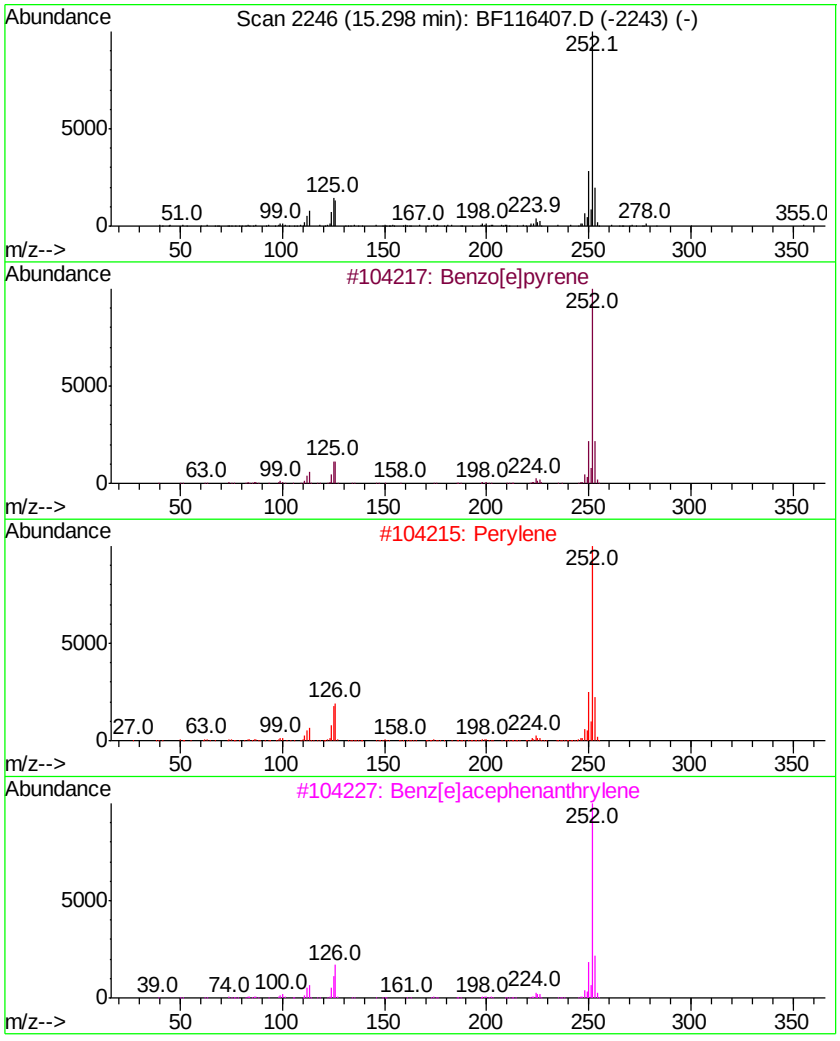
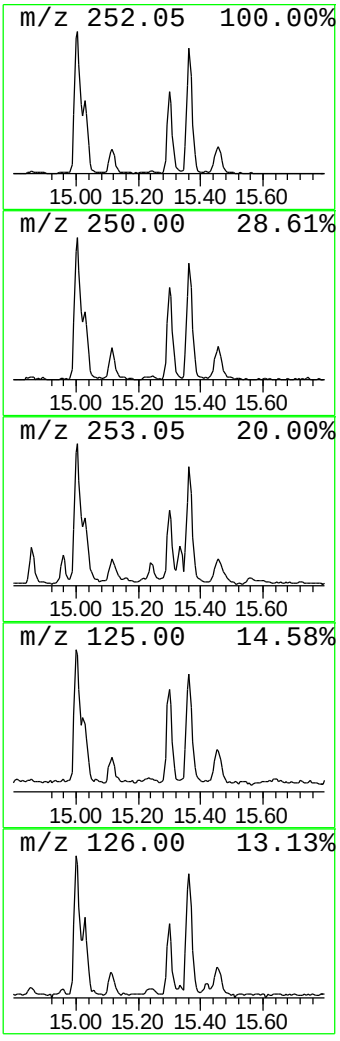
Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	5.83 ng	181188	Perylene-d12	15.42

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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\
Data File : BF116407.D
Acq On : 20 Aug 2019 00:11
Operator : HP/JU
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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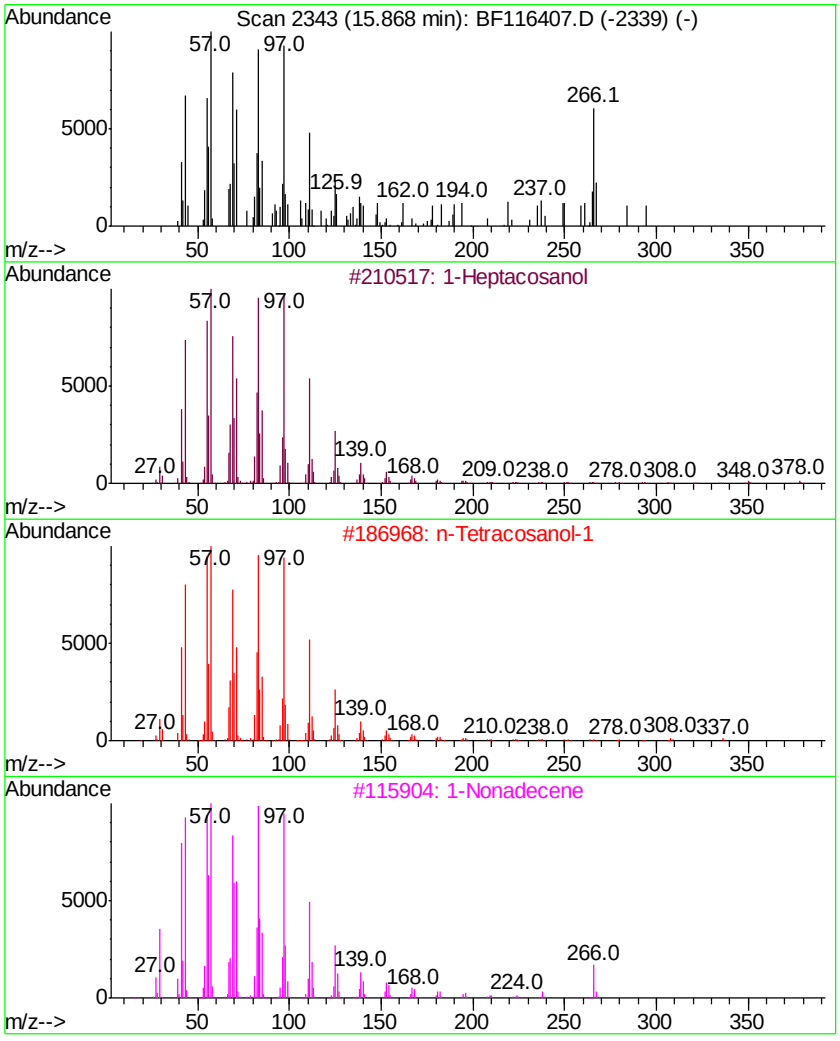
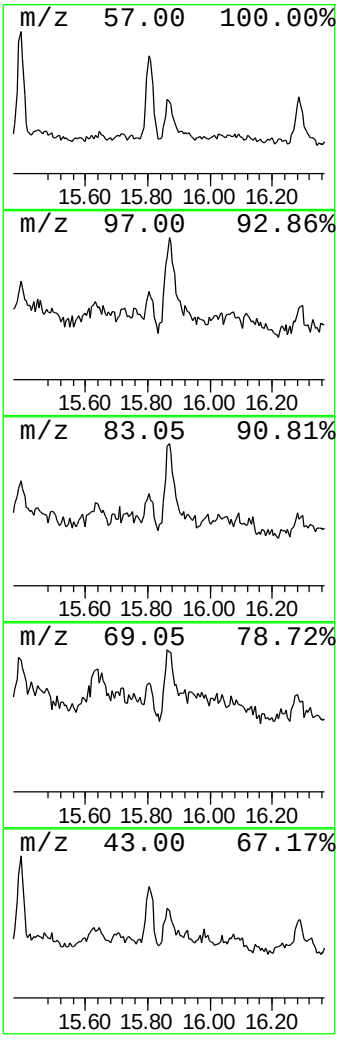
Peak Number 10 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.54 ng	78809	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	1-Nonadecene	266	C19H38	018435-45-5	87
4	Z-5-Nonadecene	266	C19H38	1000131-11-8	83
5	Octacosyl acetate	452	C30H60O2	018206-97-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081919\
Data File : BF116407.D
Acq On : 20 Aug 2019 00:11
Operator : HP/JU
Sample : K4238-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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
unknown6.58	6.58	99.1	ng	2955160	1	6.80	596451	20.0
n-Hexadecanoic acid	11.85	9.6	ng	484437	4	11.32	1011560	20.0
9-Octadecenamide,...	13.37	7.2	ng	454546	5	13.96	1270100	20.0
Benzo[c]phenanthrene	13.74	2.1	ng	131315	5	13.96	1270100	20.0
5-Octadecene, (E)-	13.78	9.1	ng	579044	5	13.96	1270100	20.0
Squalene	14.77	7.5	ng	232502	6	15.42	621149	20.0
Perylene	15.11	2.1	ng	66766	6	15.42	621149	20.0
Benzo[e]pyrene	15.30	5.8	ng	181188	6	15.42	621149	20.0
1-Heptacosanol	15.87	2.5	ng	78809	6	15.42	621149	20.0