LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116904.D
Acq On : 9 Sep 2019 18:45
Operator : HP/JU
Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

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-BF083019.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	5.451	567	572	575	rBV	1554629	1407089	71.88%	6.779%
2	6.469	740	745	764	rBV	1655516	1660034	84.81%	7.997%
3	6.604	764	768	771	rBV	1880337	1626222	83.08%	7.835%
4	6.834	803	807	816	rVB	460627	383111	19.57%	1.846%
5	6.992	830	834	837	rBV	1306333	1153335	58.92%	5.556%
6	7.392	897	902	917	rBV	1069898	982357	50.19%	4.733%
7	8.116	1021	1025	1040	rBV	516058	515341	26.33%	2.483%
8	9.186	1203	1207	1219	rBV	2069400	1857084	94.87%	8.947%
9	9.581	1270	1274	1283	rVB	180957	169857	8.68%	0.818%
10	9.869	1319	1323	1326	rBV	631938	594966	30.39%	2.866%
11	9.898	1326	1328	1339	rVB	27486	28251	1.44%	0.136%
12	10.416	1412	1416	1422	rBV	21757	23157	1.18%	0.112%
13	10.651	1452	1456	1470	rBV	1221065	1221637	62.41%	5.885%
14	11.351	1571	1575	1577	rBV	646006	633922	32.38%	3.054%
15	11.375	1577	1579	1584	rVV	294540	254650	13.01%	1.227%
16	11.422	1584	1587	1591	rVB	52394	54378	2.78%	0.262%
17	11.580	1608	1614	1619	rBV2	23775	37492	1.92%	0.181%
18	11.851	1655	1660	1661	rBV	35805	31454	1.61%	0.152%
19	11.874	1661	1664	1670	rVB3	145537	138342	7.07%	0.666%
20	11.963	1675	1679	1681	rVV	69843	73500	3.75%	0.354%
21	11.986	1681	1683	1687	rVB	26308	22722	1.16%	0.109%
22	12.169	1712	1714	1719	rVB	28882	25710	1.31%	0.124%
23	12.398	1749	1753	1754	rBV	25536	25541	1.30%	0.123%
24	12.433	1754	1759	1765	rVV4	42870	92290	4.71%	0.445%
25	12.480	1765	1767	1772	rVB3	27249	31173	1.59%	0.150%
26	12.557	1776	1780	1784	rBV	509173	463965	23.70%	2.235%
27	12.657	1794	1797	1801	rBV	75039	72395	3.70%	0.349%
28	12.786	1814	1819	1825	rVB	453479	466574	23.84%	2.248%
29	12.933	1839	1844	1847	rBV	2069593	1957466	100.00%	9.430%
30	13.004	1851	1856	1860	rBV2	28210	46670	2.38%	0.225%
31	13.092	1868	1871	1872	rBV3	29774	29939	1.53%	0.144%
32	13.110	1872	1874	1878	rVB	54604	56145	2.87%	0.270%
33	13.180	1883	1886	1889	rVV	46578	36792	1.88%	0.177%
34	13.216	1889	1892	1895	rVV	34588	35006	1.79%	0.169%

LSC Area Percent Report

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Sample : K4755-01
Misc :
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Instrument : BNA_F
ClientSampleId : RO-1-3

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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.310	1905	1908	1911	rBV	35762	31756	1.62%	0.153%
36	13.339	1911	1913	1917	rBV2	24104	27785	1.42%	0.134%
37	13.621	1958	1961	1966	rVB	38636	40920	2.09%	0.197%
38	13.733	1973	1980	1982	rBV3	38566	53415	2.73%	0.257%
39	13.780	1986	1988	1992	rVV2	39503	58115	2.97%	0.280%
40	13.845	1993	1999	2013	rVB7	105609	323808	16.54%	1.560%
41	13.980	2015	2022	2025	rBV3	695885	954566	48.77%	4.599%
42	14.004	2025	2026	2034	rVB	194236	182887	9.34%	0.881%
43	14.086	2038	2040	2042	rBV	28087	24114	1.23%	0.116%
44	14.145	2047	2050	2053	rVV	38589	41431	2.12%	0.200%
45	14.198	2057	2059	2063	rBV2	21180	27966	1.43%	0.135%
46	14.368	2084	2088	2091	rBV	40588	49305	2.52%	0.238%
47	14.404	2091	2094	2097	rBV3	29475	26188	1.34%	0.126%
48	14.451	2097	2102	2107	rBV4	78716	88897	4.54%	0.428%
49	14.498	2107	2110	2112	rBV3	44030	42424	2.17%	0.204%
50	14.568	2117	2122	2126	rVB4	22397	27710	1.42%	0.133%
51	14.757	2150	2154	2157	rBV	123072	119885	6.12%	0.578%
52	14.833	2163	2167	2170	rBV	63579	72057	3.68%	0.347%
53	15.015	2194	2198	2202	rBV	275501	424475	21.68%	2.045%
54	15.086	2206	2210	2214	rVV2	137090	165951	8.48%	0.799%
55	15.121	2214	2216	2221	rVB	36834	39260	2.01%	0.189%
56	15.215	2227	2232	2237	rBV3	16659	35237	1.80%	0.170%
57	15.315	2245	2249	2255	rVB	154586	202470	10.34%	0.975%
58	15.374	2255	2259	2265	rBV	168146	229772	11.74%	1.107%
59	15.439	2265	2270	2273	rBV	427107	595254	30.41%	2.868%
60	15.886	2342	2346	2355	rVB	98626	156410	7.99%	0.754%
61	16.386	2426	2431	2439	rVB	58305	97253	4.97%	0.469%
62	16.880	2509	2515	2523	rBV2	83434	162194	8.29%	0.781%
63	16.962	2524	2529	2539	rVB6	25761	60049	3.07%	0.289%
64	17.051	2539	2544	2550	rBV5	14531	30872	1.58%	0.149%
65	17.121	2550	2556	2557	rBV5	11977	22876	1.17%	0.110%
66	17.315	2582	2589	2597	rVB2	63185	133249	6.81%	0.642%

Sum of corrected areas: 20757118

LSC Report - Integrated Chromatogram

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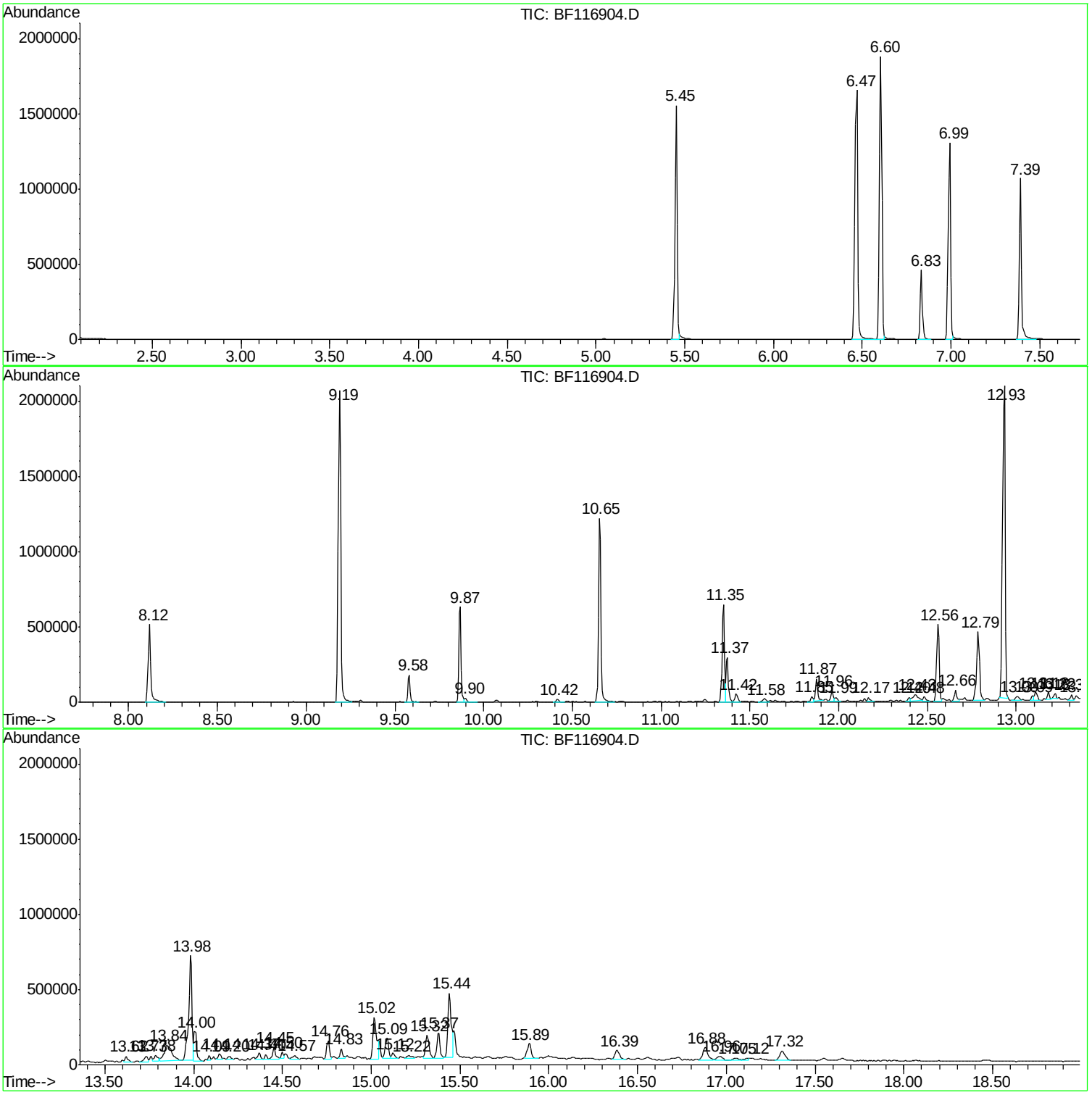
Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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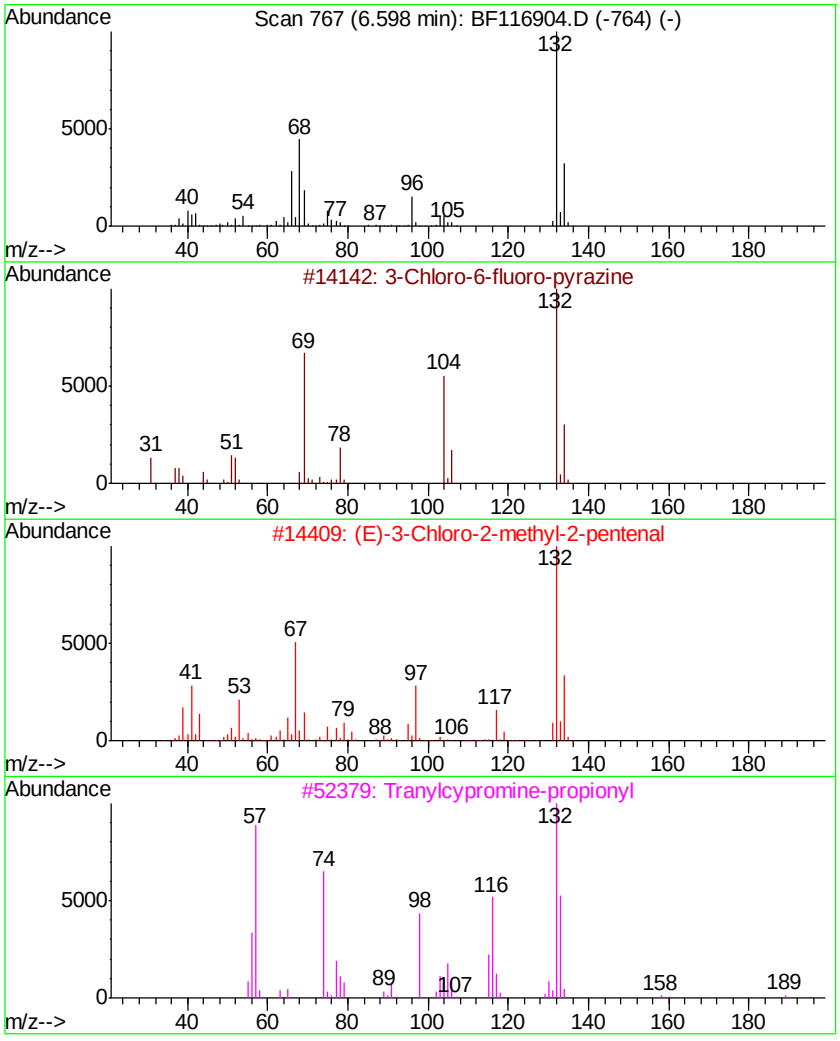
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

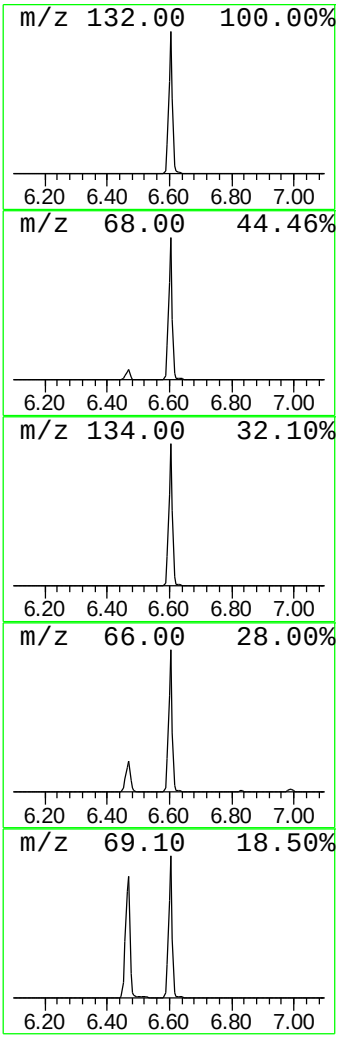
****

Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	84.90 ng	1626220	1,4-Dichlorobenzene-d4	6.83

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Data File : BF116904.D
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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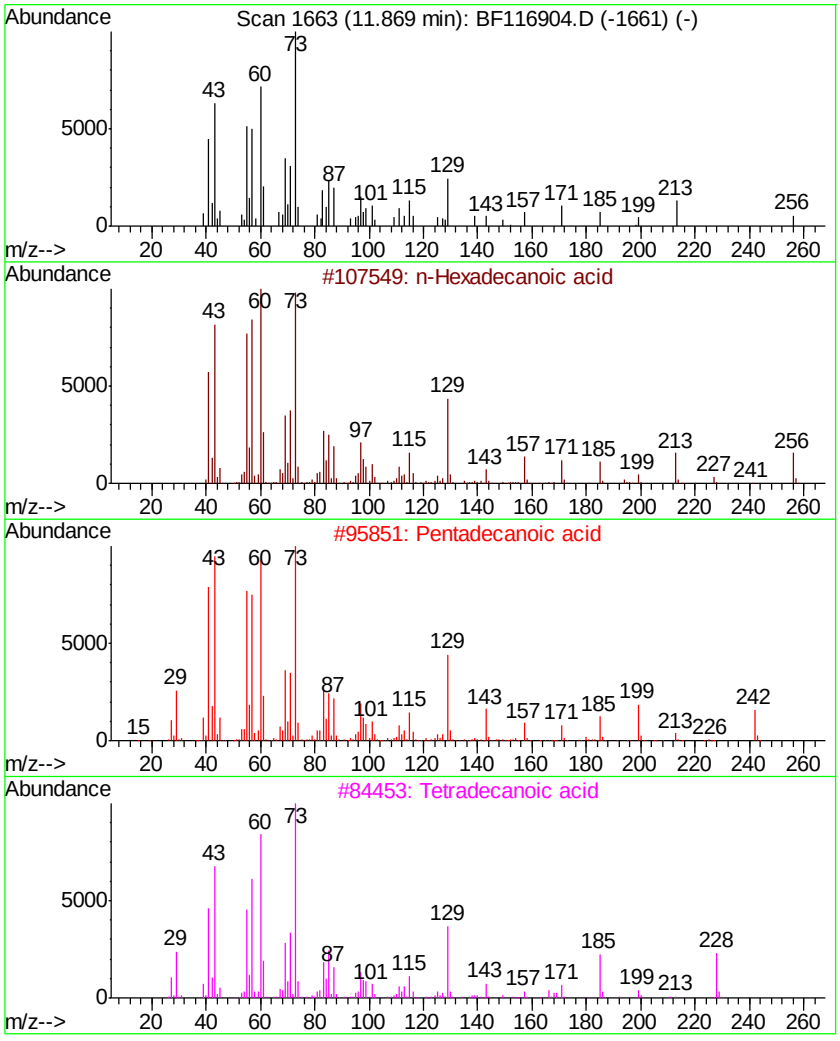
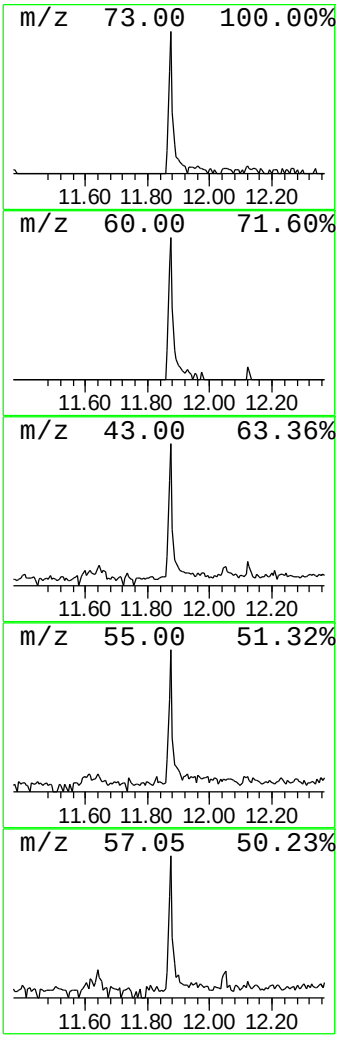
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.36 ng	138342	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
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Acq On : 9 Sep 2019 18:45
Operator : HP/JU
Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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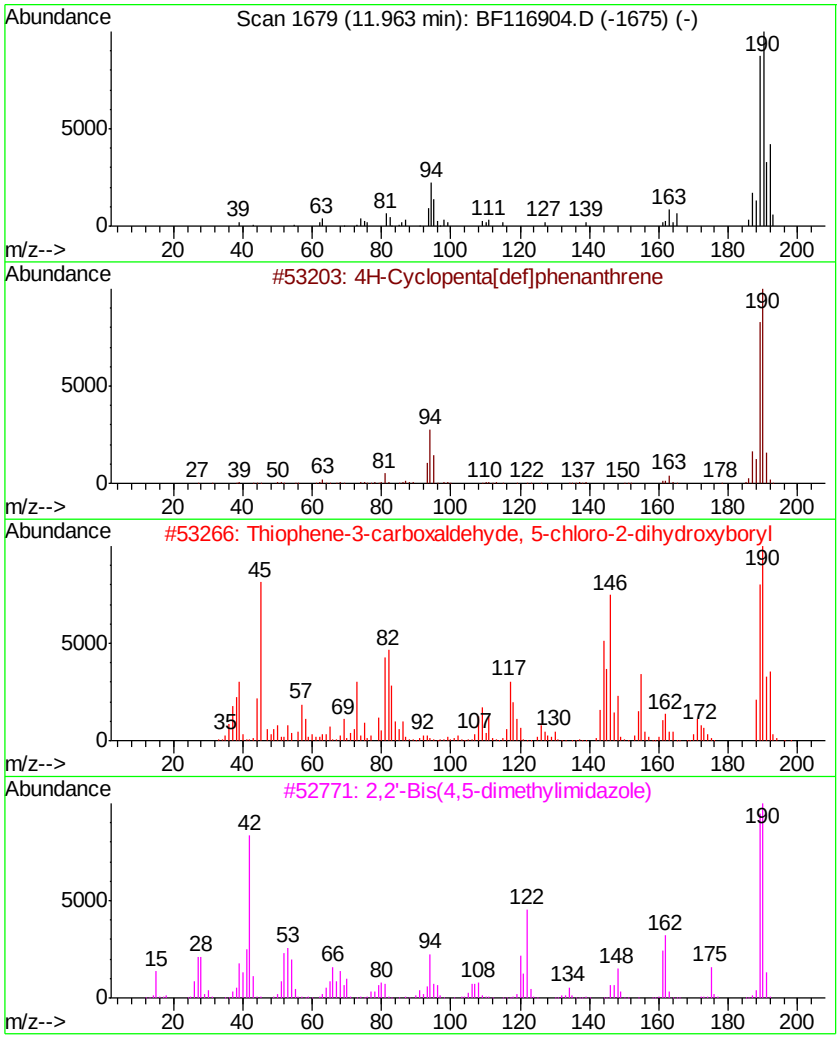
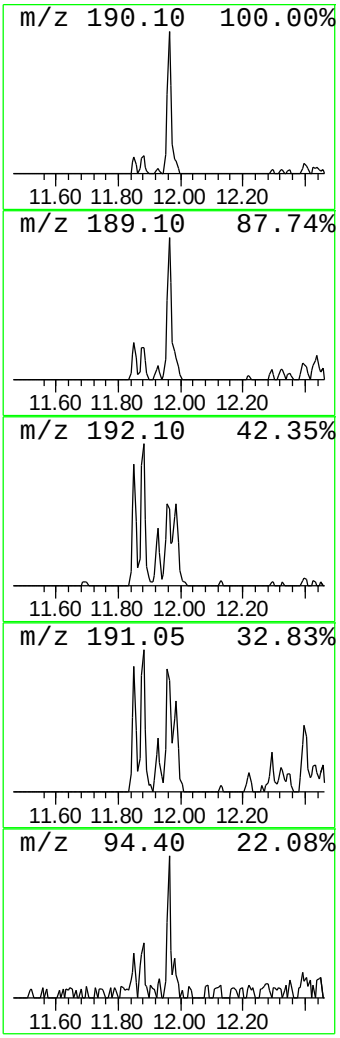
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.32 ng	73500	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	38
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	38





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : RO-1-3

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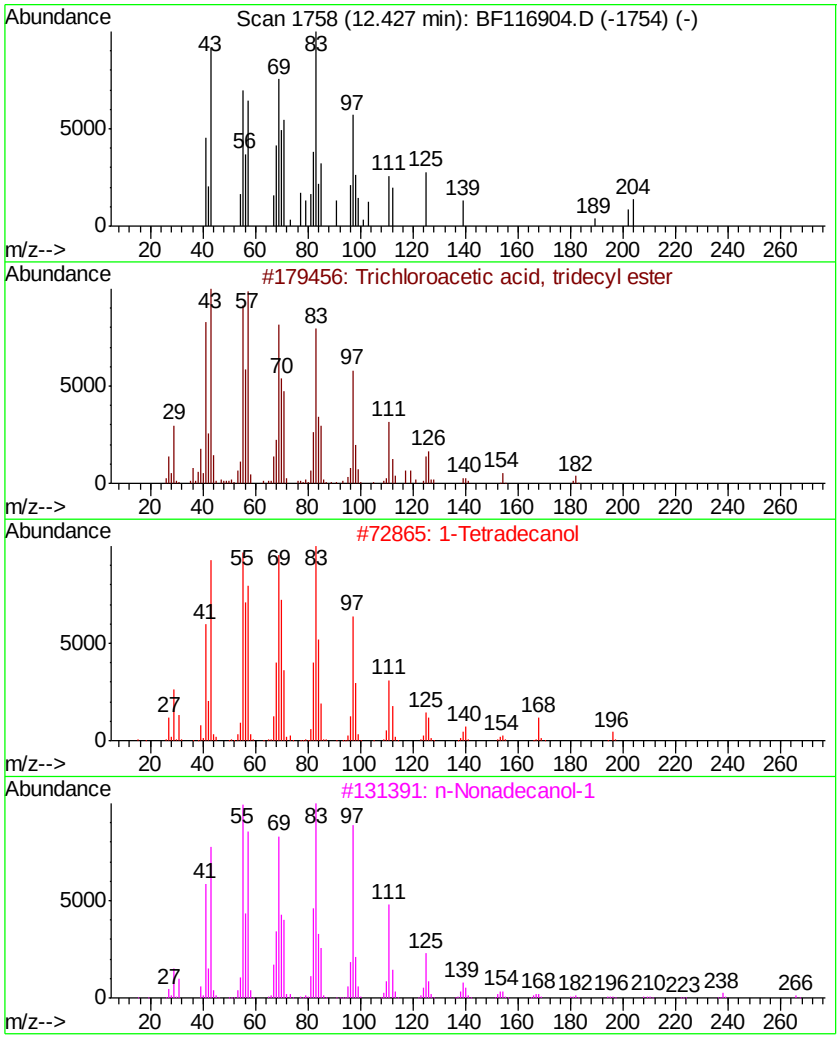
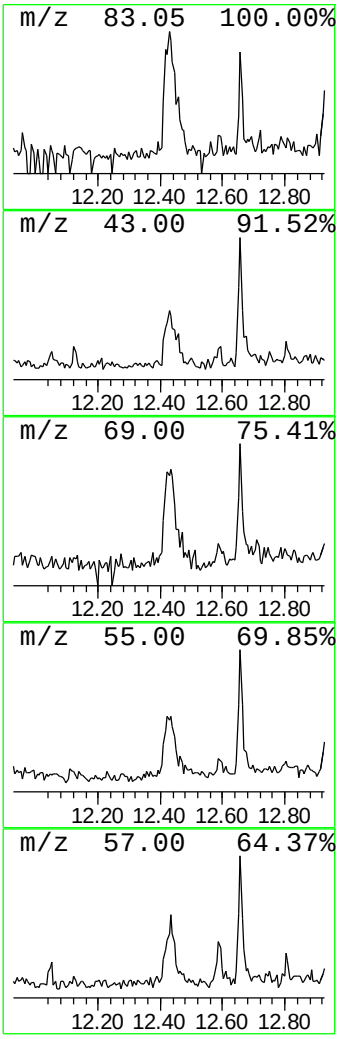
Peak Number 5 Trichloroacetic acid, tride... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	2.91 ng	92290	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	70
2	1-Tetradecanol	214	C14H30O	000112-72-1	52
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	47
4	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	46
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	46





Library Search Compound Report

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Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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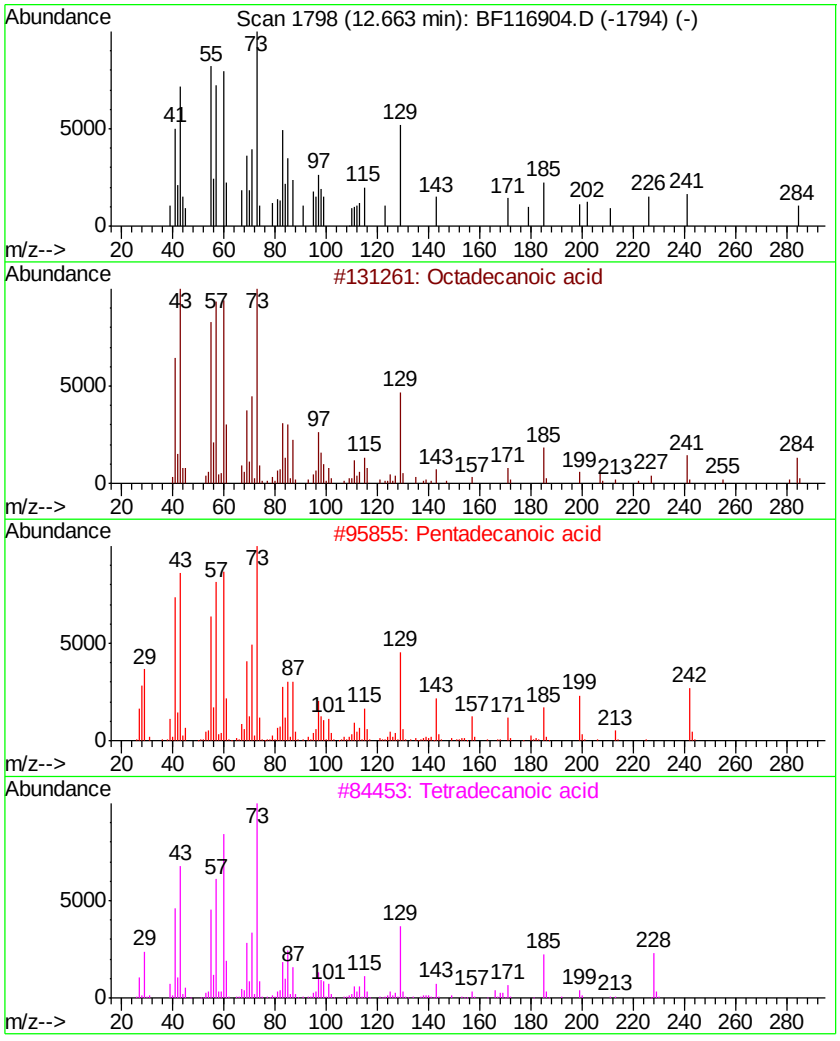
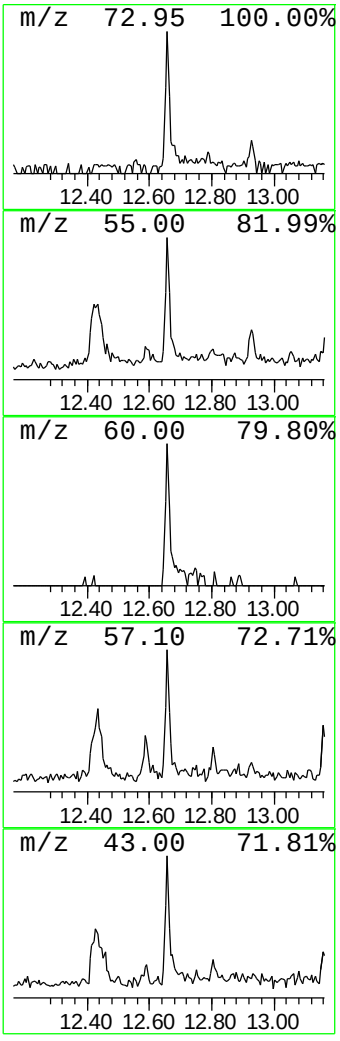
Peak Number 6 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	2.28 ng	72395	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
5	Dodecanoic acid	200	C12H24O2	000143-07-7	45





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Instrument : BNA_F
ClientSampleId : RO-1-3

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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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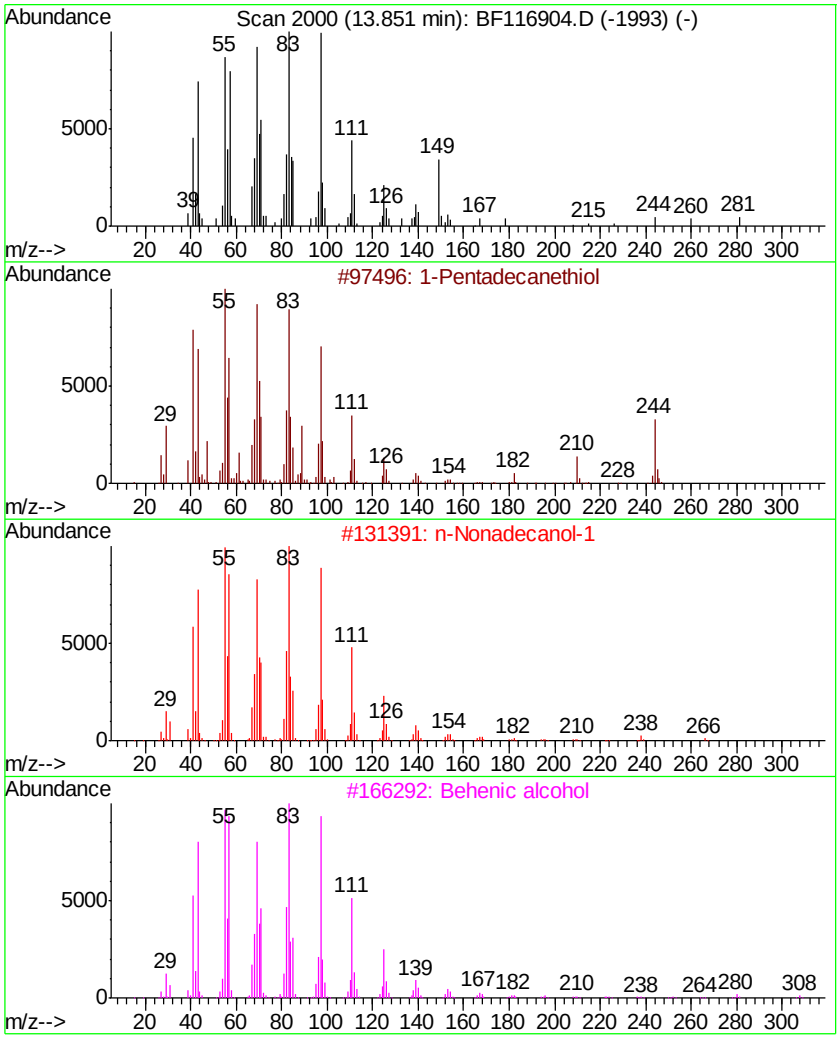
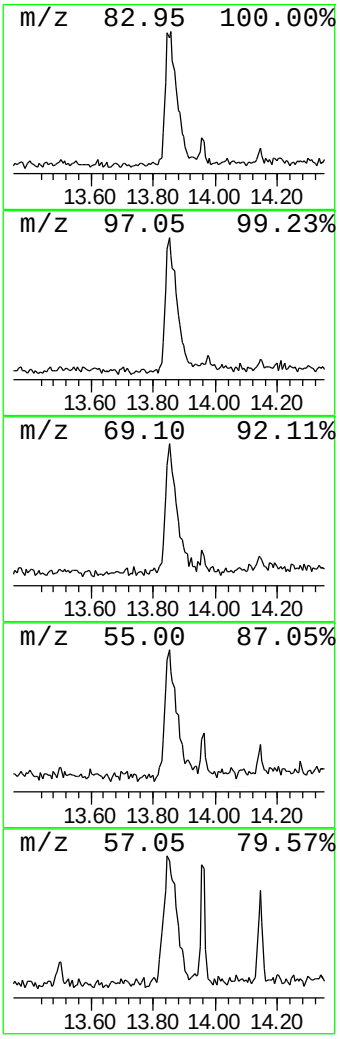
Peak Number 7 1-Pentadecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	6.78 ng	323808	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	87
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	87





Library Search Compound Report

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Data File : BF116904.D
Acq On : 9 Sep 2019 18:45
Operator : HP/JU
Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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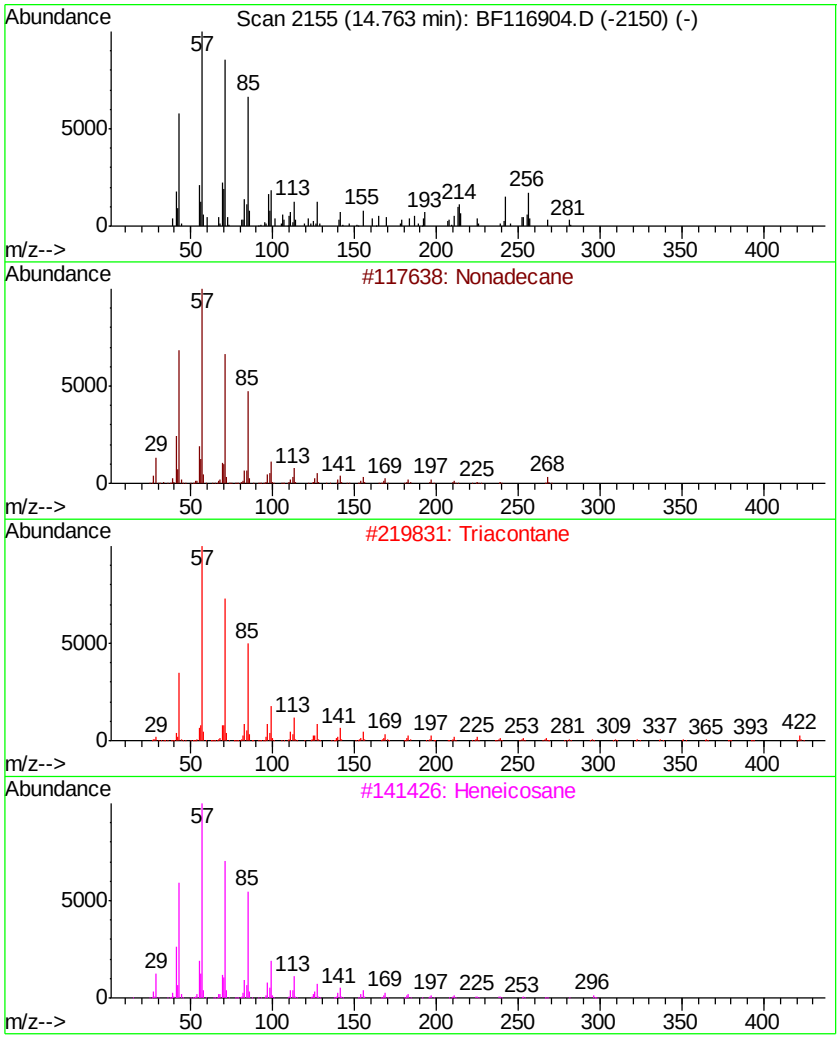
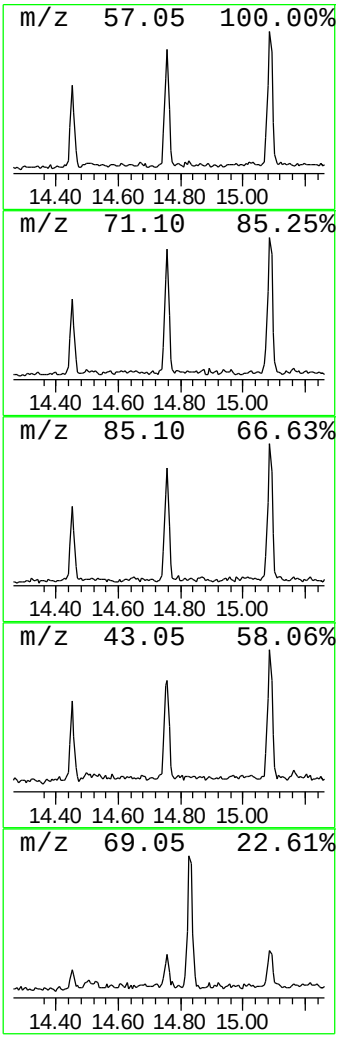
Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	4.03 ng	119885	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Triacontane	422	C30H62	000638-68-6	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Hexadecane	226	C16H34	000544-76-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116904.D
Acq On : 9 Sep 2019 18:45
Operator : HP/JU
Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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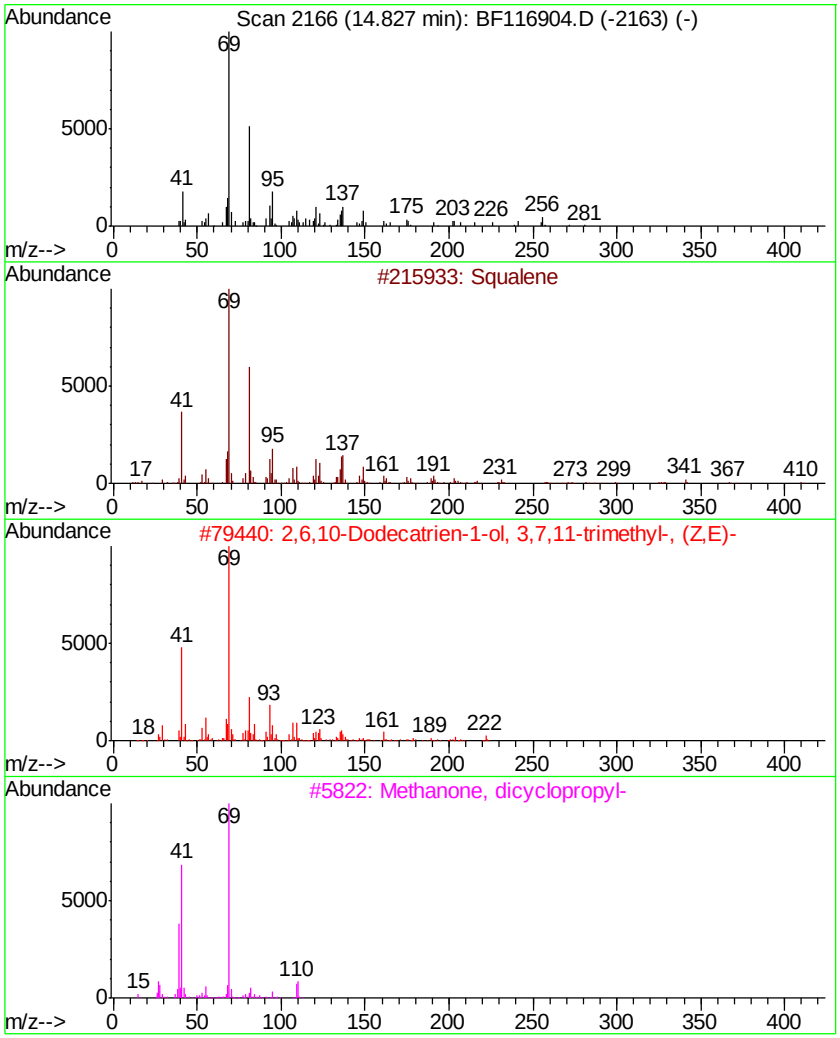
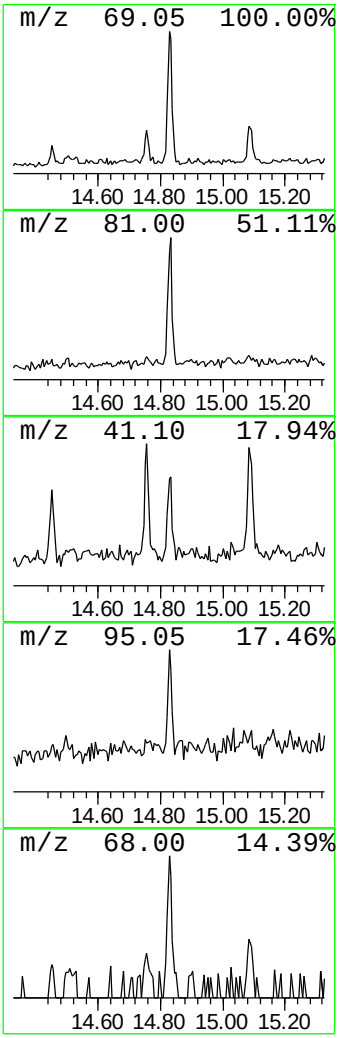
Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.42 ng	72057	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	53
3	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	50
4	2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	50
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116904.D
Acq On : 9 Sep 2019 18:45
Operator : HP/JU
Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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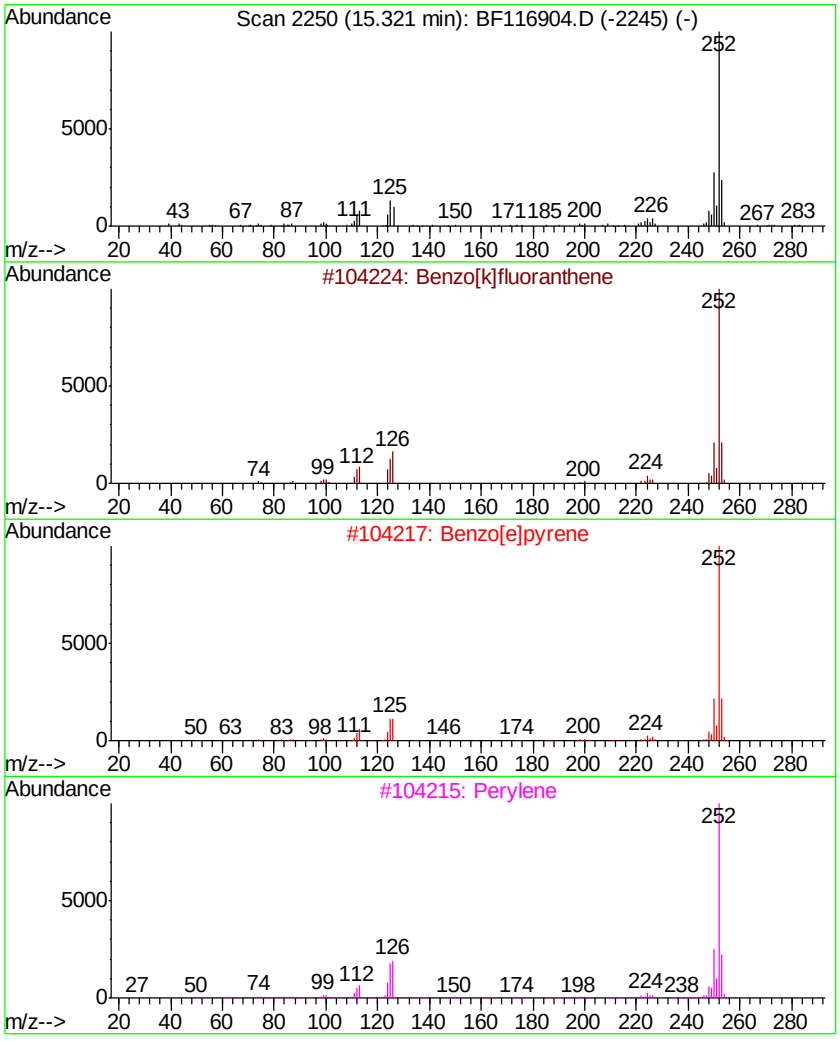
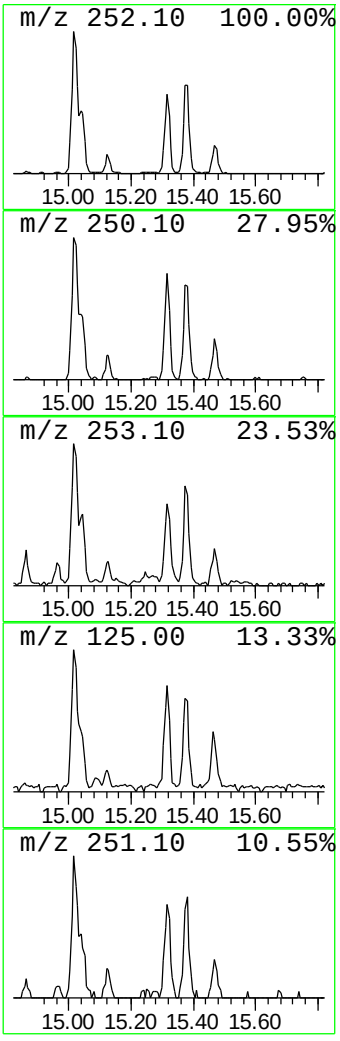
Peak Number 10 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	6.80 ng	202470	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	96
3	Perylene	252	C20H12	000198-55-0	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Library Search Compound Report

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Data File : BF116904.D
Acq On : 9 Sep 2019 18:45
Operator : HP/JU
Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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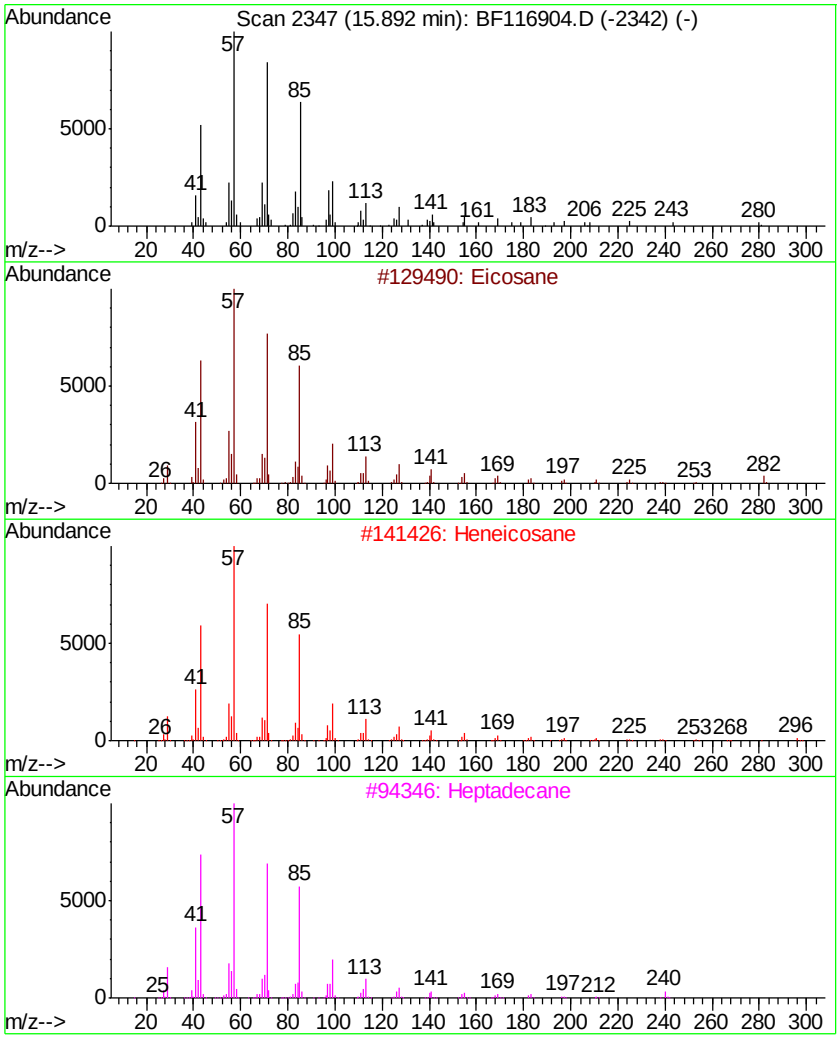
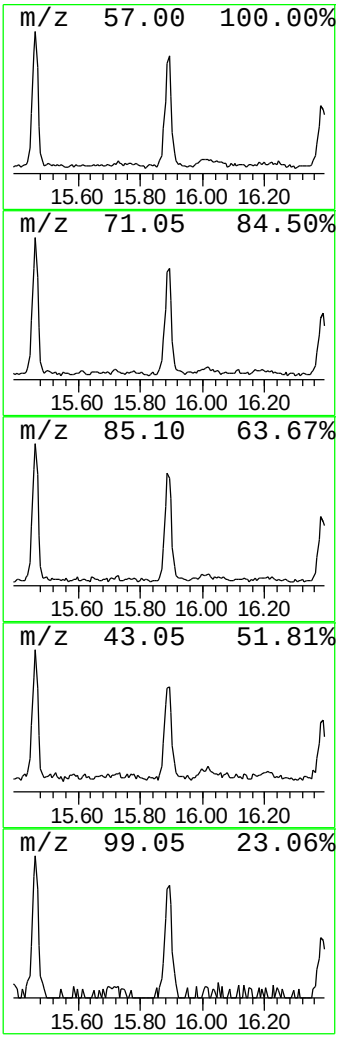
Peak Number 11 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	5.26 ng	156410	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Acq On : 9 Sep 2019 18:45
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Sample : K4755-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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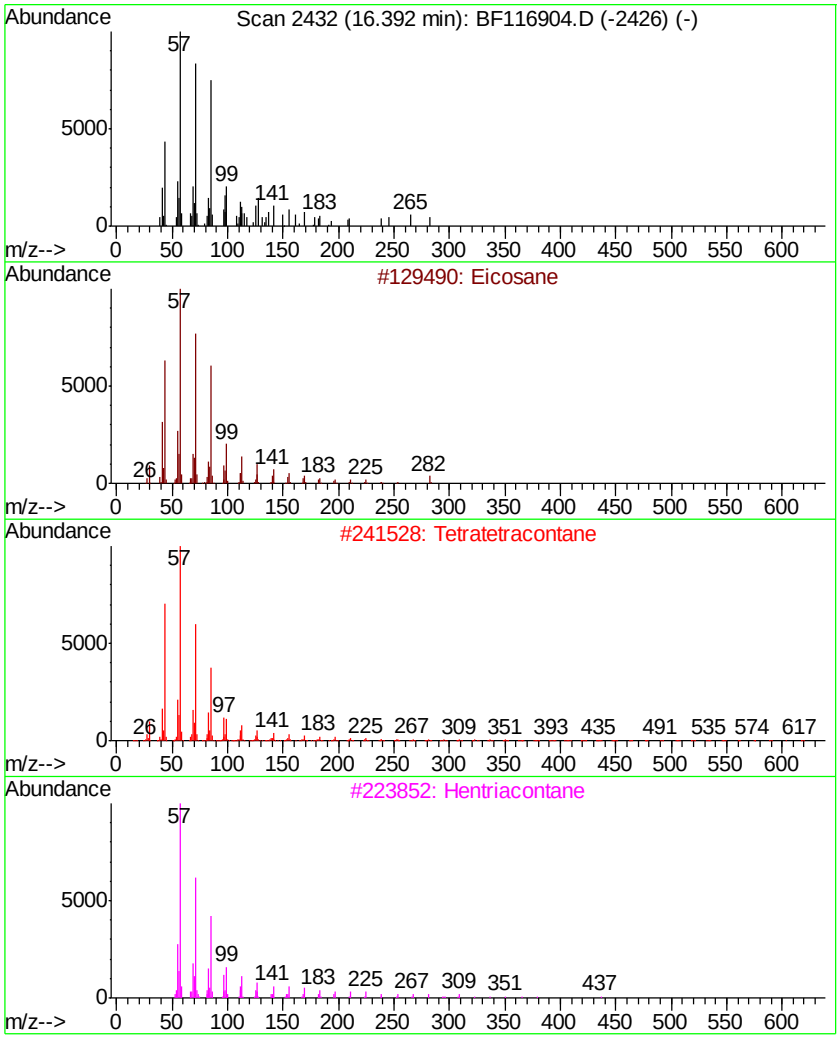
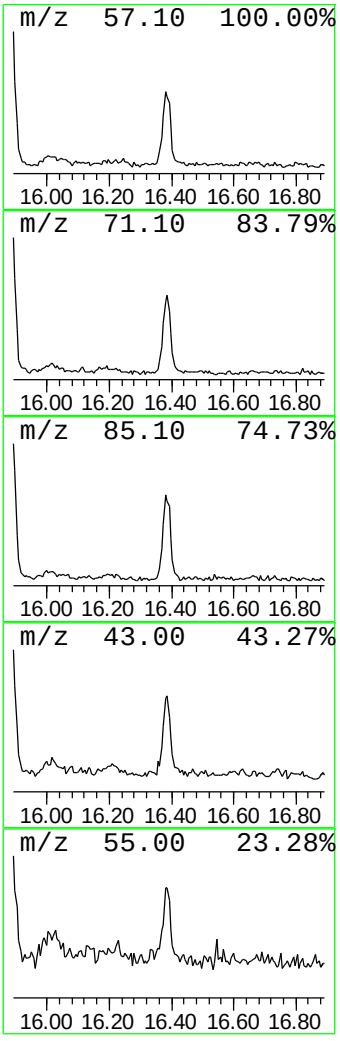
Peak Number 12 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.39	3.27 ng	97253	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	2-methyltetracosane	352	C25H52	1000376-72-6	83
5	2-methyloctacosane	408	C29H60	1000376-72-8	83





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-1-3

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TIC Library : C:\DATABASE\NIST11.L
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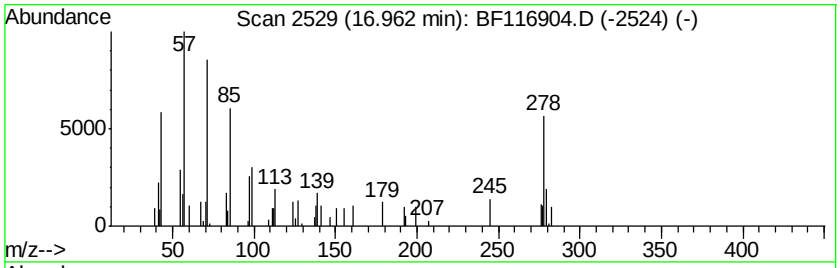
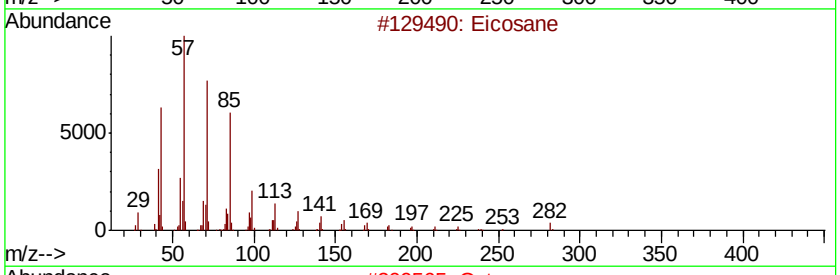
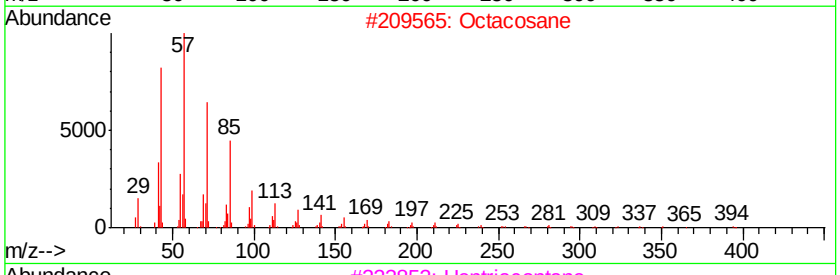
Peak Number 13 Eicosane Concentration Rank 13

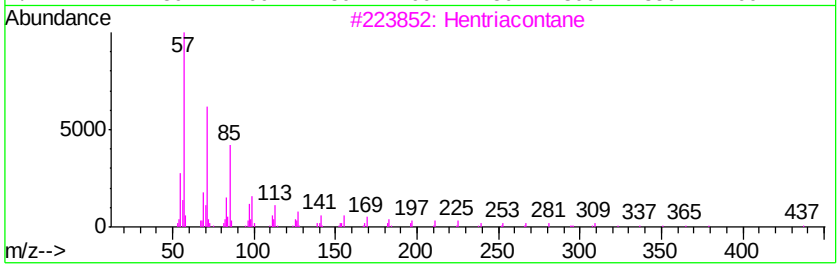
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	2.02 ng	60049	Perylene-d12	15.44

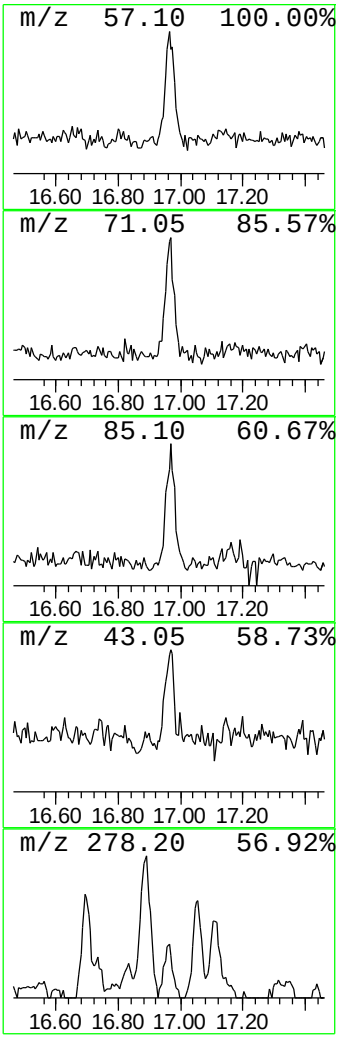
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	60
2	Octacosane	394	C28H58	000630-02-4	46
3	Hentriacontane	437	C31H64	000630-04-6	46
4	2-methyloctacosane	408	C29H60	1000376-72-8	46
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	43











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090919\
Data File : BF116904.D
Acq On : 9 Sep 2019 18:45
Operator : HP/JU
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.60	6.60	84.9	ng	1626220	1	6.83	383111	20.0
n-Hexadecanoic acid	11.87	4.4	ng	138342	4	11.35	633922	20.0
4H-Cyclopenta[def...	11.96	2.3	ng	73500	4	11.35	633922	20.0
Trichloroacetic a...	12.43	2.9	ng	92290	4	11.35	633922	20.0
Octadecanoic acid	12.66	2.3	ng	72395	4	11.35	633922	20.0
1-Pentadecanethiol	13.85	6.8	ng	323808	5	13.99	954566	20.0
Nonadecane	14.76	4.0	ng	119885	6	15.44	595254	20.0
Squalene	14.83	2.4	ng	72057	6	15.44	595254	20.0
Benzo[e]pyrene	15.32	6.8	ng	202470	6	15.44	595254	20.0
Heneicosane	15.89	5.3	ng	156410	6	15.44	595254	20.0
Tetratetracontane	16.39	3.3	ng	97253	6	15.44	595254	20.0
Eicosane	16.96	2.0	ng	60049	6	15.44	595254	20.0