LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081719\
Data File : BF116367.D
Acq On : 17 Aug 2019 19:40
Operator : HP/JU
Sample : K4223-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-10

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	3.875	300	304	321	rVB	24592	45027	1.50%	0.129%
2	5.439	566	570	599	rBV	2537177	2824334	94.08%	8.078%
3	6.451	739	742	755	rBV	2563097	3002091	100.00%	8.587%
4	6.586	761	765	772	rVB	2926841	2967846	98.86%	8.489%
5	6.810	800	803	811	rBV	955296	853096	28.42%	2.440%
6	6.963	826	829	840	rVB	2427073	2256068	75.15%	6.453%
7	7.375	895	899	909	rBV	2015422	1913255	63.73%	5.472%
8	8.069	1014	1017	1018	rBV	50811	43641	1.45%	0.125%
9	8.086	1018	1020	1029	rVV	1122936	1093143	36.41%	3.127%
10	8.145	1029	1030	1033	rVB	40578	30967	1.03%	0.089%
11	8.380	1063	1070	1076	rBV7	22003	36024	1.20%	0.103%
12	8.504	1088	1091	1094	rBV	39278	41356	1.38%	0.118%
13	8.675	1117	1120	1124	rBV	37592	32430	1.08%	0.093%
14	9.104	1190	1193	1199	rBV	36357	30365	1.01%	0.087%
15	9.163	1199	1203	1206	rBV	3085605	2875789	95.79%	8.225%
16	9.239	1213	1216	1219	rVB	42853	40534	1.35%	0.116%
17	9.557	1266	1270	1274	rBV	656083	566530	18.87%	1.620%
18	9.839	1314	1318	1322	rBV	1475204	1253968	41.77%	3.587%
19	9.957	1335	1338	1341	rVB	47766	42496	1.42%	0.122%
20	10.633	1449	1453	1468	rBV	1931089	1962889	65.38%	5.614%
21	10.751	1468	1473	1476	rBV4	39781	53168	1.77%	0.152%
22	10.992	1512	1514	1522	rBV5	36723	52939	1.76%	0.151%
23	11.327	1567	1571	1573	rBV	1287804	1118374	37.25%	3.199%
24	11.351	1573	1575	1580	rVV	246388	252570	8.41%	0.722%
25	11.410	1583	1585	1590	rVB	36223	37569	1.25%	0.107%
26	11.580	1610	1614	1617	rVB2	46088	44897	1.50%	0.128%
27	11.780	1644	1648	1651	rBV	209789	279975	9.33%	0.801%
28	11.857	1657	1661	1668	rVB2	608482	695434	23.16%	1.989%
29	11.945	1673	1676	1678	rBV	67388	61500	2.05%	0.176%
30	12.010	1685	1687	1692	rVB	83023	76219	2.54%	0.218%
31	12.121	1704	1706	1709	rBV	38010	36321	1.21%	0.104%
32	12.380	1747	1750	1752	rBV2	45165	40693	1.36%	0.116%
33	12.410	1752	1755	1758	rVB4	38869	48726	1.62%	0.139%
34	12.468	1762	1765	1774	rVB4	58887	97579	3.25%	0.279%

LSC Area Percent Report

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Instrument : BNA_F
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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	12.545	1774	1778	1780	rBV	426450	476107	15.86%	1.362%
36	12.568	1780	1782	1787	rVB	190762	189050	6.30%	0.541%
37	12.633	1790	1793	1801	rBV2	140056	183026	6.10%	0.523%
38	12.692	1801	1803	1805	rBV2	41242	34269	1.14%	0.098%
39	12.721	1805	1808	1811	rBV2	63376	66895	2.23%	0.191%
40	12.768	1811	1816	1823	rVV	416206	580946	19.35%	1.662%
41	12.827	1823	1826	1835	rVV7	56014	125830	4.19%	0.360%
42	12.904	1835	1839	1843	rVB	2469476	2148389	71.56%	6.145%
43	13.086	1867	1870	1871	rBV3	30286	34651	1.15%	0.099%
44	13.104	1871	1873	1875	rVB	44575	37214	1.24%	0.106%
45	13.204	1888	1890	1895	rVB3	43577	52244	1.74%	0.149%
46	13.298	1903	1906	1909	rBV3	73033	89917	3.00%	0.257%
47	13.333	1909	1912	1917	rVV3	75564	109146	3.64%	0.312%
48	13.404	1921	1924	1925	rBV	74574	66109	2.20%	0.189%
49	13.792	1987	1990	2002	rVB2	345176	527009	17.55%	1.507%
50	13.968	2015	2020	2023	rBV2	903175	981002	32.68%	2.806%
51	13.998	2023	2025	2032	rVB	161327	174143	5.80%	0.498%
52	14.110	2042	2044	2047	rBV2	40618	47747	1.59%	0.137%
53	14.415	2094	2096	2102	rVB3	117939	179005	5.96%	0.512%
54	14.786	2157	2159	2164	rVB	80913	77011	2.57%	0.220%
55	15.009	2193	2197	2199	rBV	176629	221276	7.37%	0.633%
56	15.039	2199	2202	2206	rVB2	450727	460433	15.34%	1.317%
57	15.309	2245	2248	2251	rVB	90296	97534	3.25%	0.279%
58	15.368	2255	2258	2262	rBV	111049	120728	4.02%	0.345%
59	15.427	2264	2268	2273	rVB	569113	714427	23.80%	2.043%
60	15.827	2331	2336	2341	rVB	284227	415829	13.85%	1.189%
61	17.327	2585	2591	2594	rBV6	64363	163087	5.43%	0.466%
62	17.386	2596	2601	2616	rVB7	219735	822474	27.40%	2.352%
63	17.827	2672	2676	2685	rBV4	85775	261334	8.71%	0.747%
64	17.915	2688	2691	2705	rVB6	154668	440686	14.68%	1.260%
65	18.156	2727	2732	2737	rBV5	107694	256858	8.56%	0.735%

Sum of corrected areas: 34962189

LSC Report - Integrated Chromatogram

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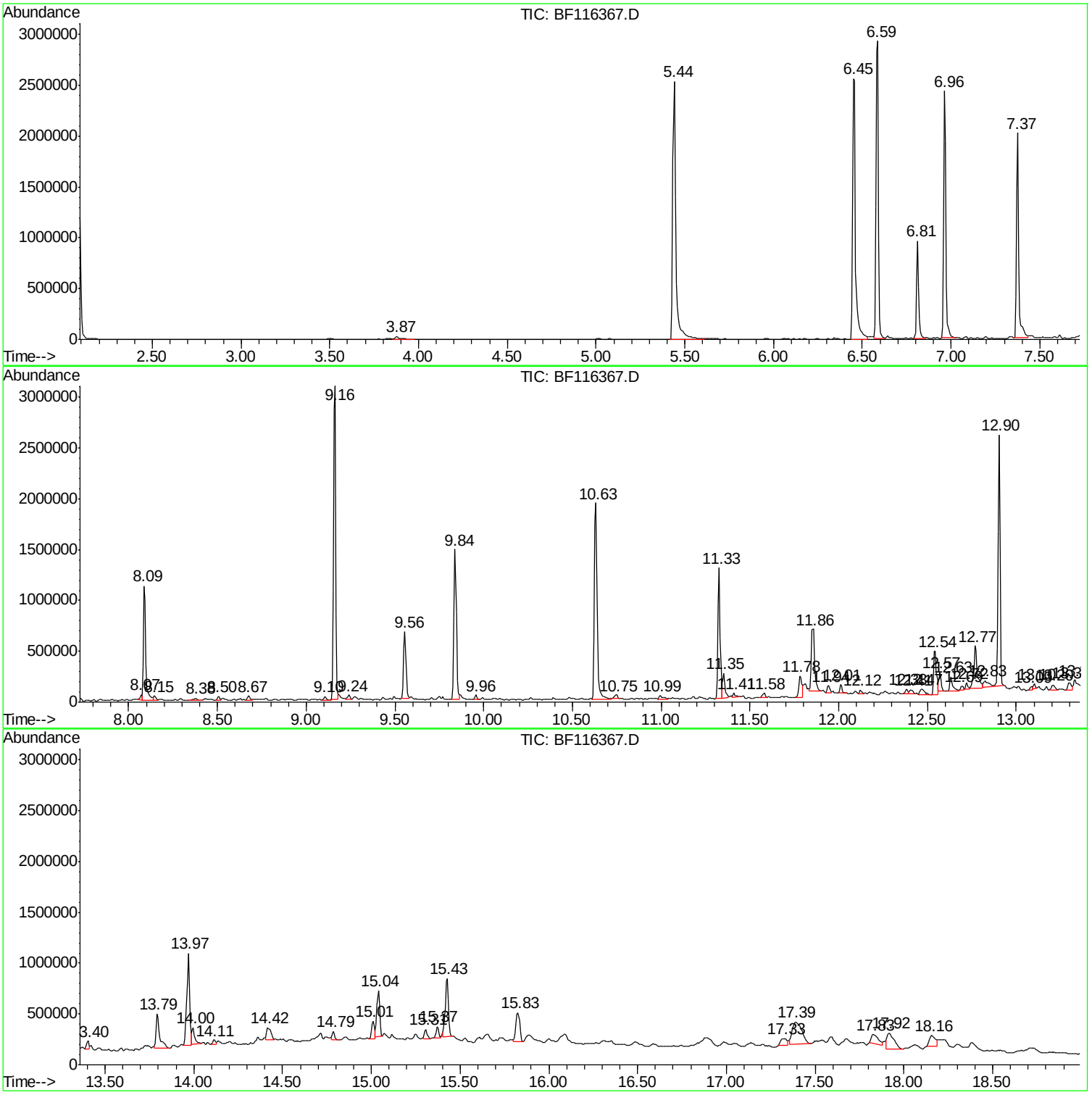
Instrument : BNA_F
ClientSampleId : SP-10

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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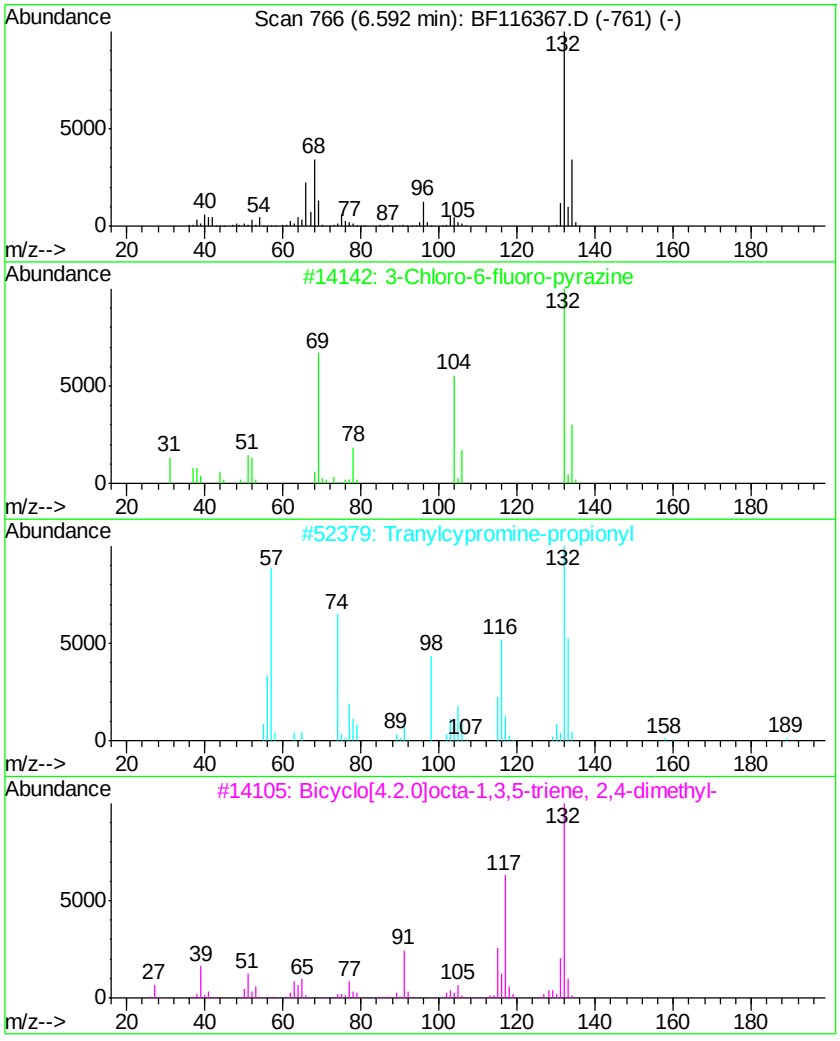
TIC Integration Parameters: LSCINT.P

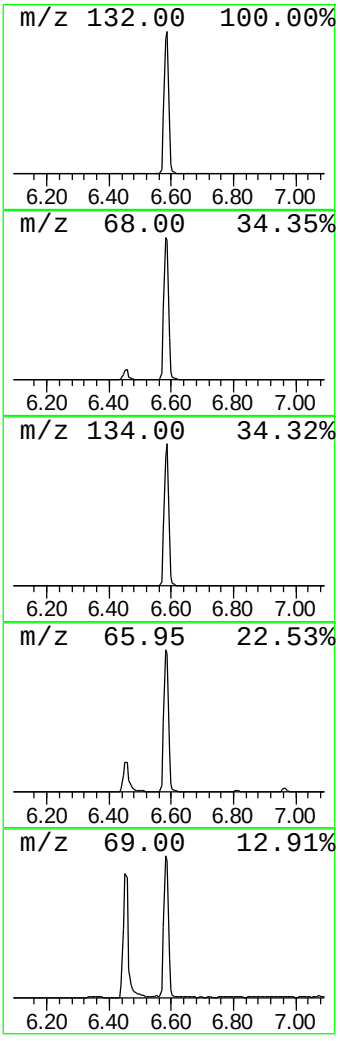
****

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	69.58 ng	2967850	1,4-Dichlorobenzene-d4	6.81

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : SP-10

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

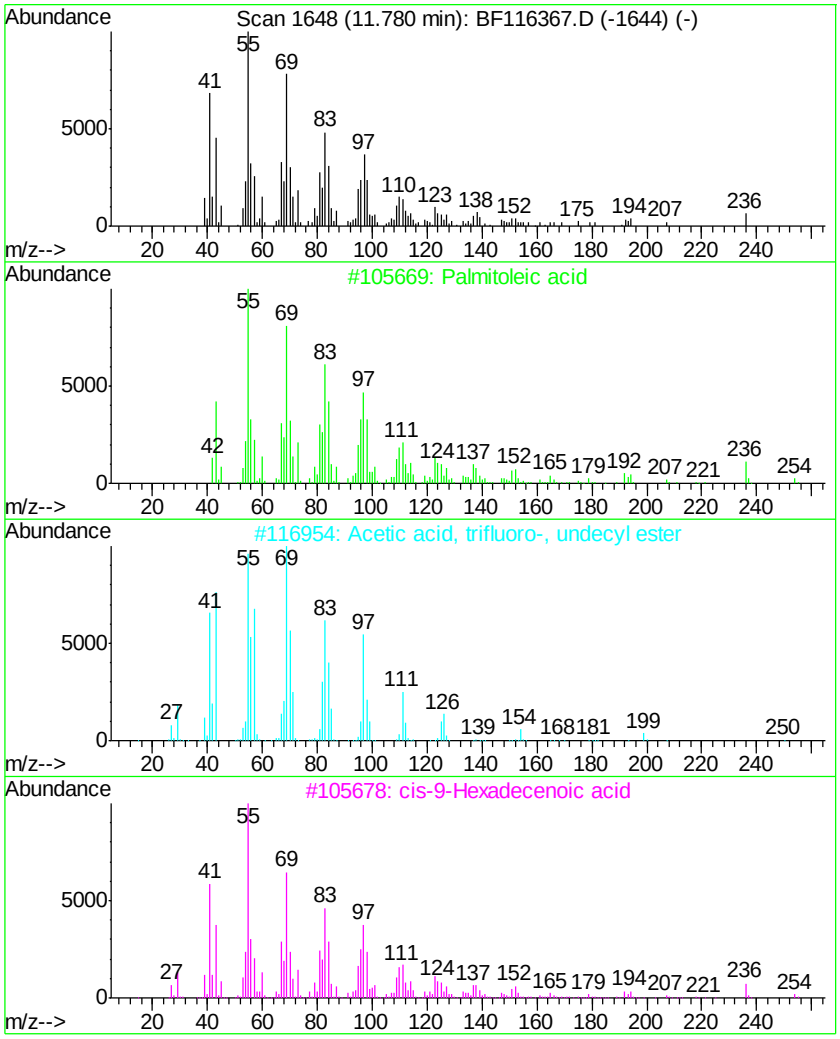
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

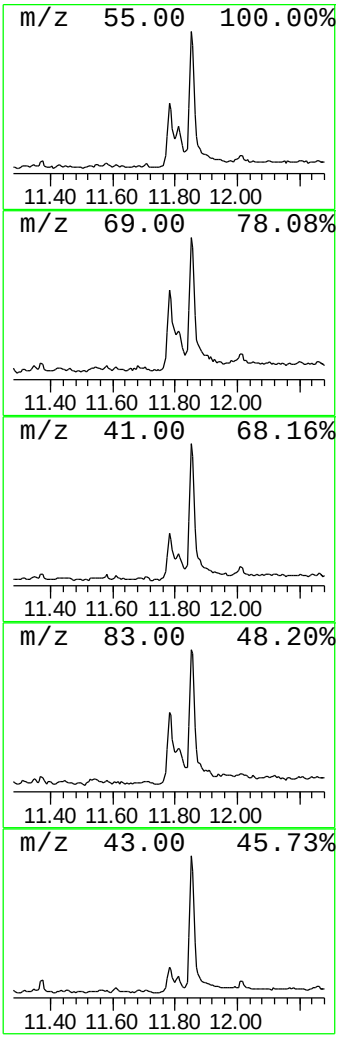
****

Peak Number 3 Palmitoleic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	5.01 ng	279975	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	91
2	Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	70
3	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	64
4	1-Cyclohexyl-2-methyl-prop-2-en-...	152	C10H16O	025183-82-8	64
5	Cyclobutanone, 2-(1,1-dimethylet...	126	C8H14O	004579-31-1	53





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
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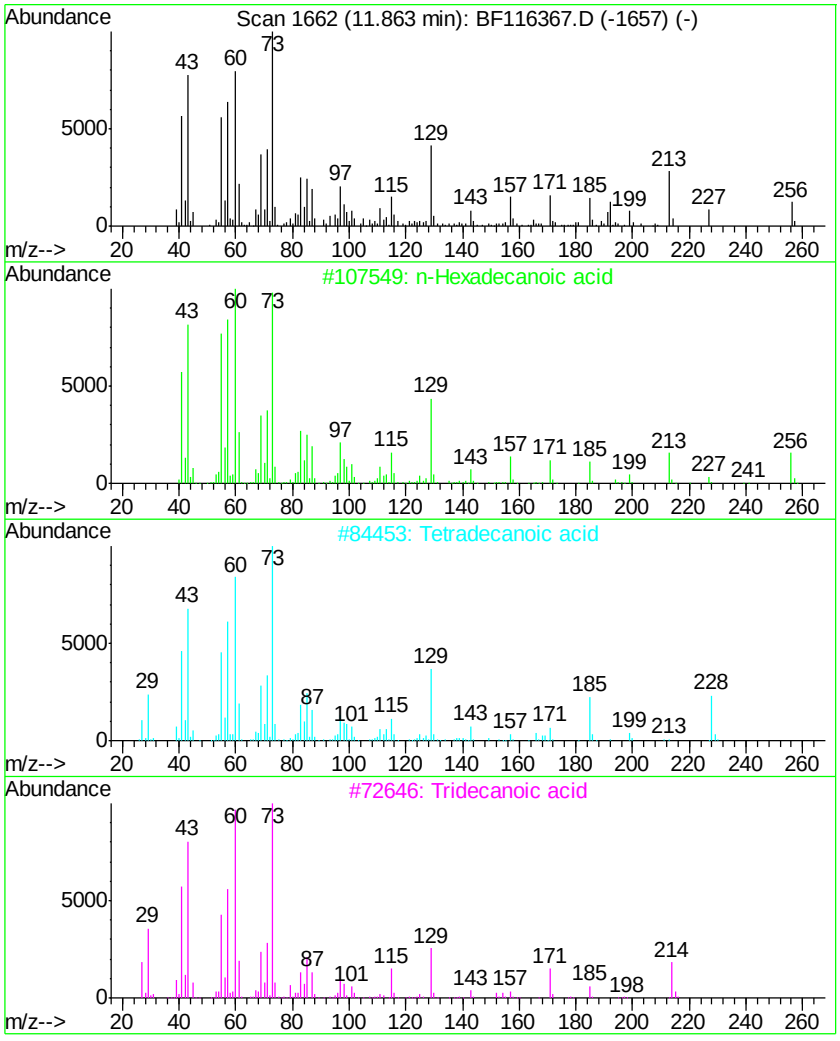
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

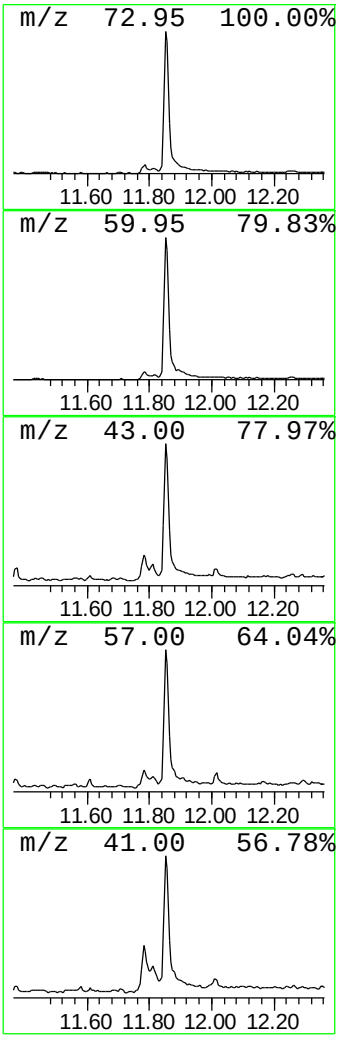
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	12.44 ng	695434	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-10

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TIC Library : C:\DATABASE\NIST11.L
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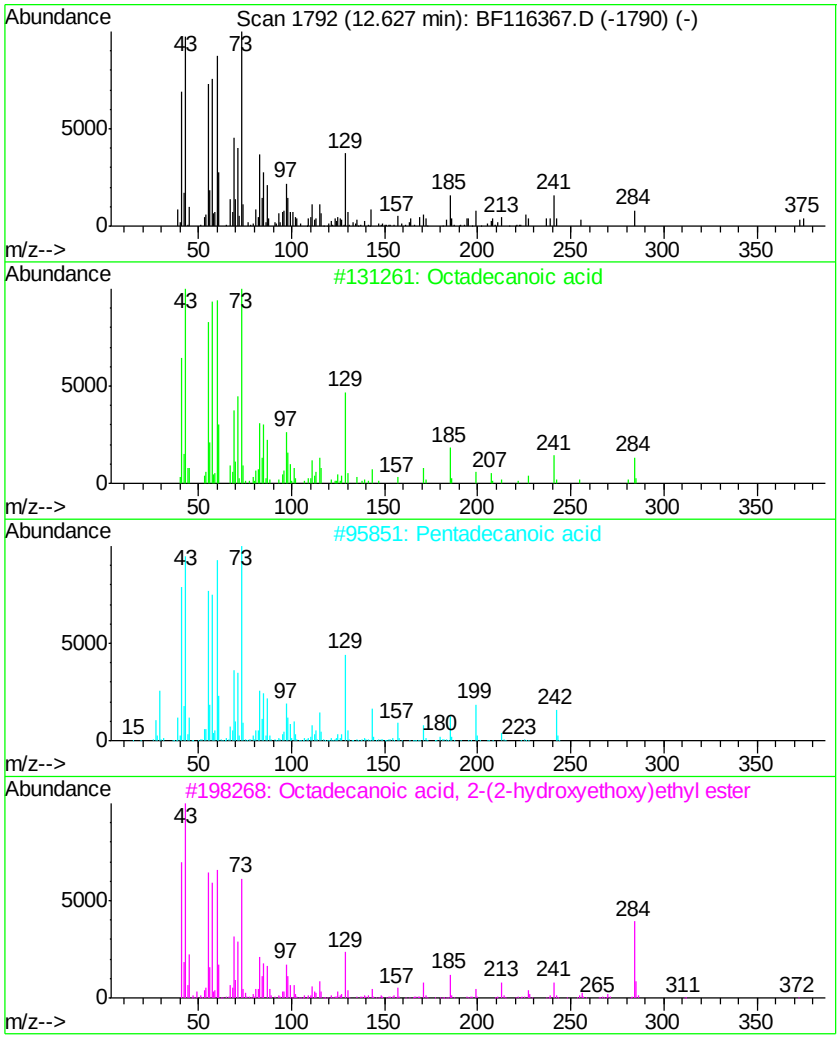
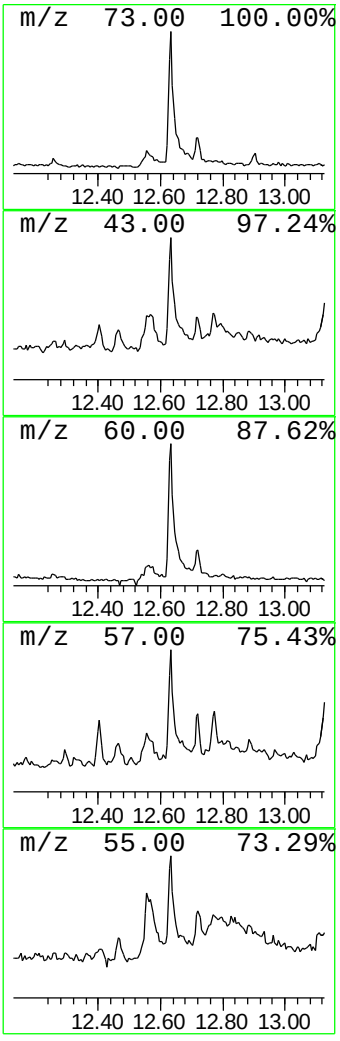
****

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	3.27 ng	183026	Phenanthrene-d10	11.33

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	94
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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

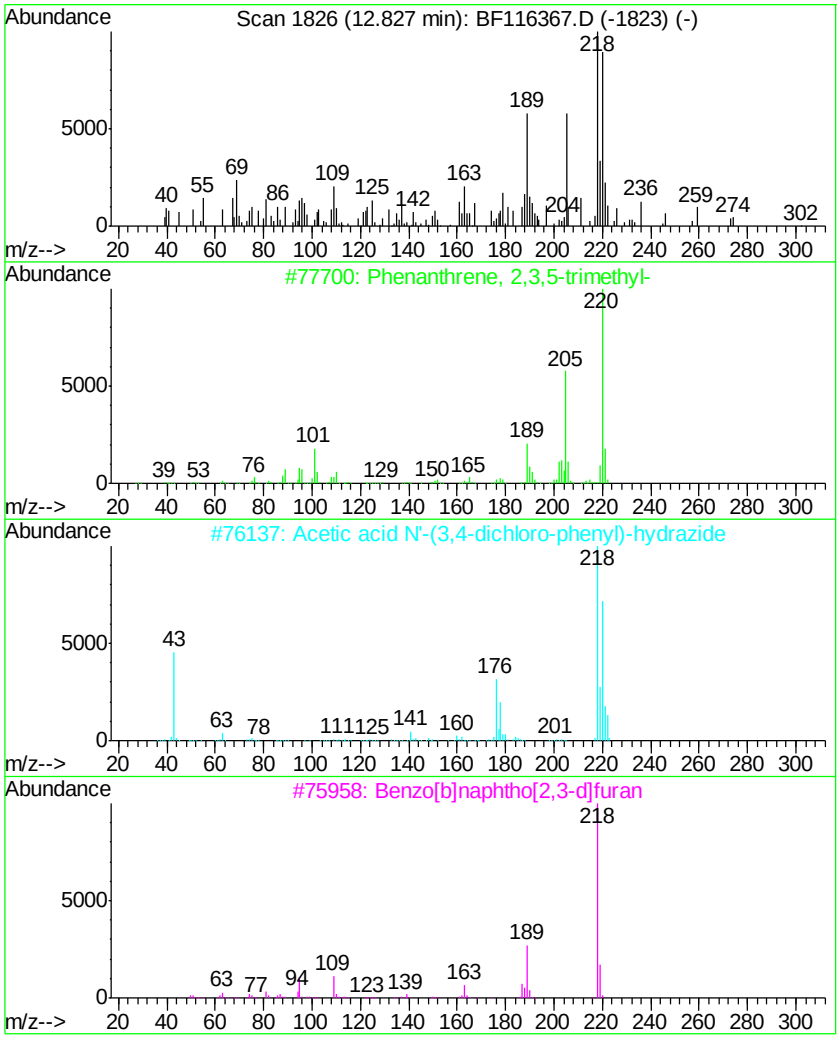
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

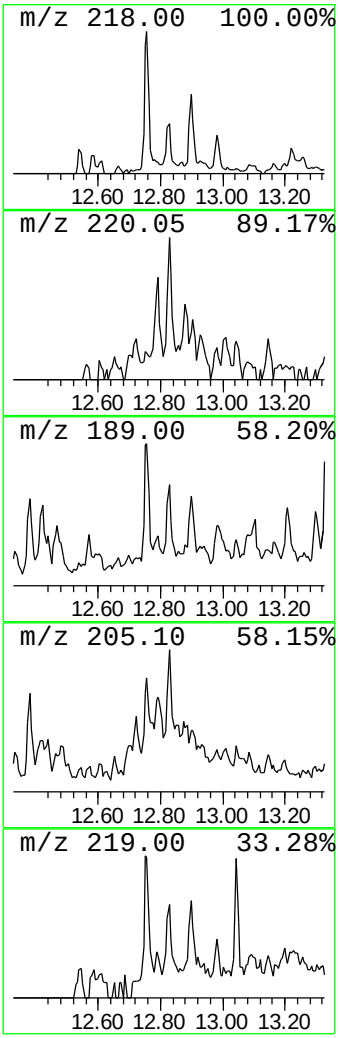
****

Peak Number 6 Phenanthrene, 2,3,5-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.57 ng	125830	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,3,5-trimethyl-	220	C17H16	003674-73-5	50
2	Acetic acid N'-(3,4-dichloro-phe...	218	C8H8Cl2N2O	1000294-80-9	47
3	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	46
4	10-Methylanthracene-9-carboxalde...	220	C16H12O	007072-00-6	43
5	Xylazine	220	C12H16N2S	007361-61-7	38





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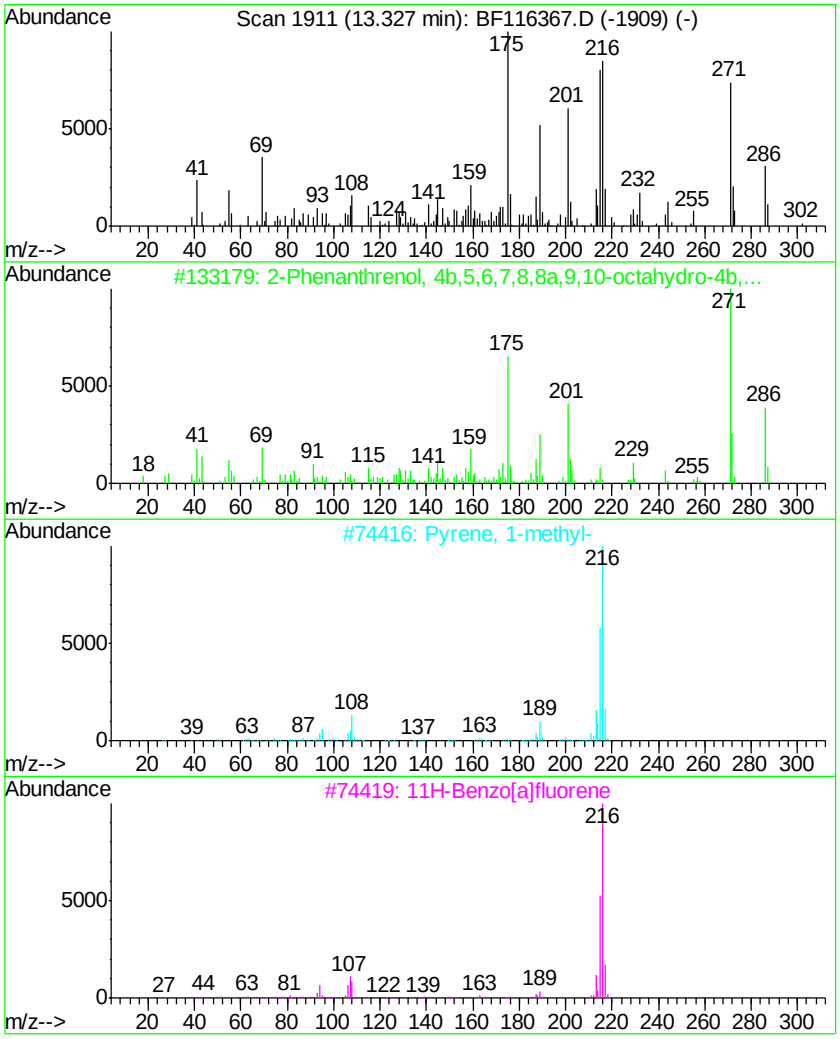
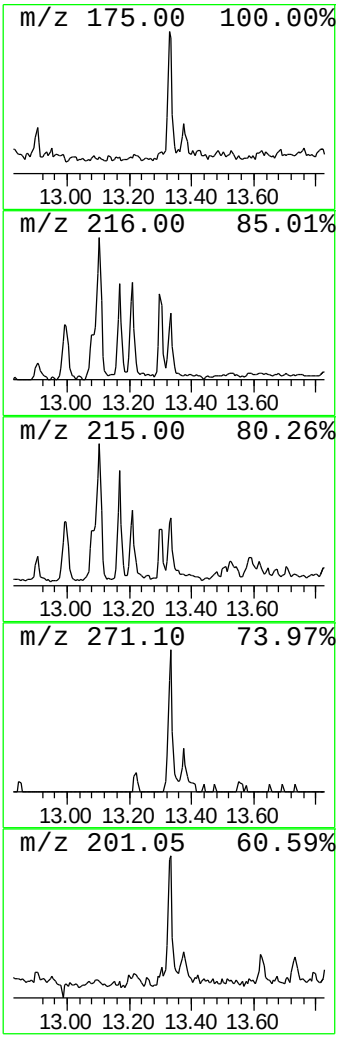
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	2.23 ng	109146	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	86
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	70
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	38
4	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	38
5	Pyrene, 4-methyl-	216	C17H12	003353-12-6	35





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-10

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

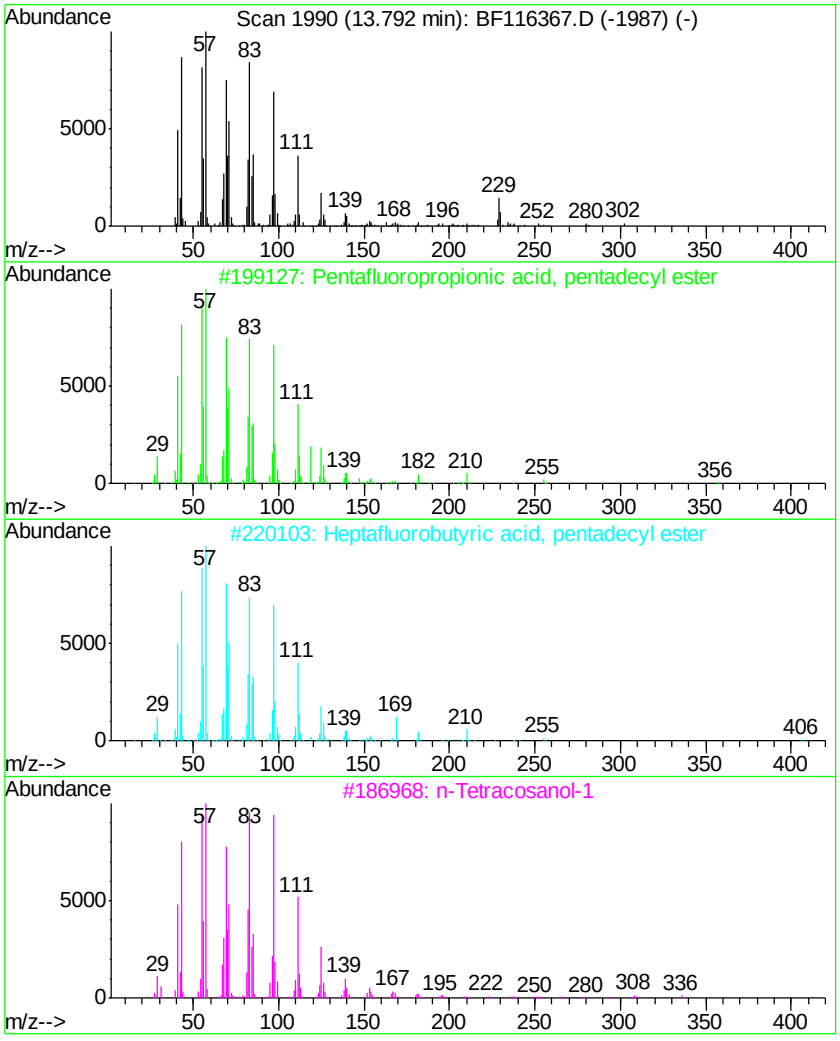
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

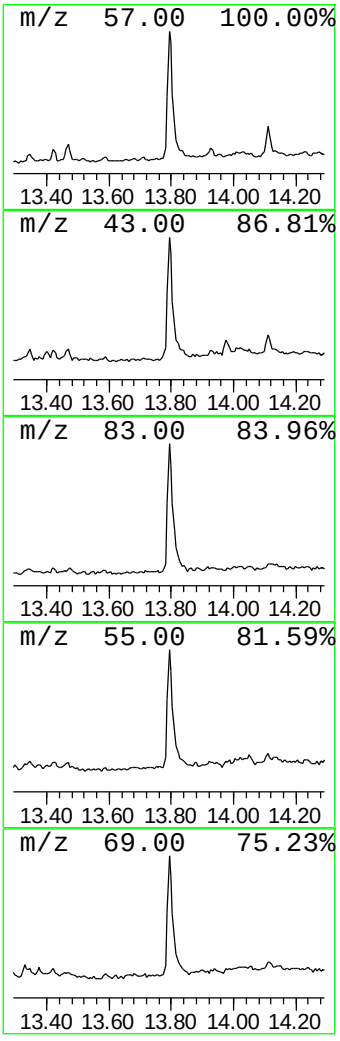
****

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	10.74 ng	527009	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081719\
Data File : BF116367.D
Acq On : 17 Aug 2019 19:40
Operator : HP/JU
Sample : K4223-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-10

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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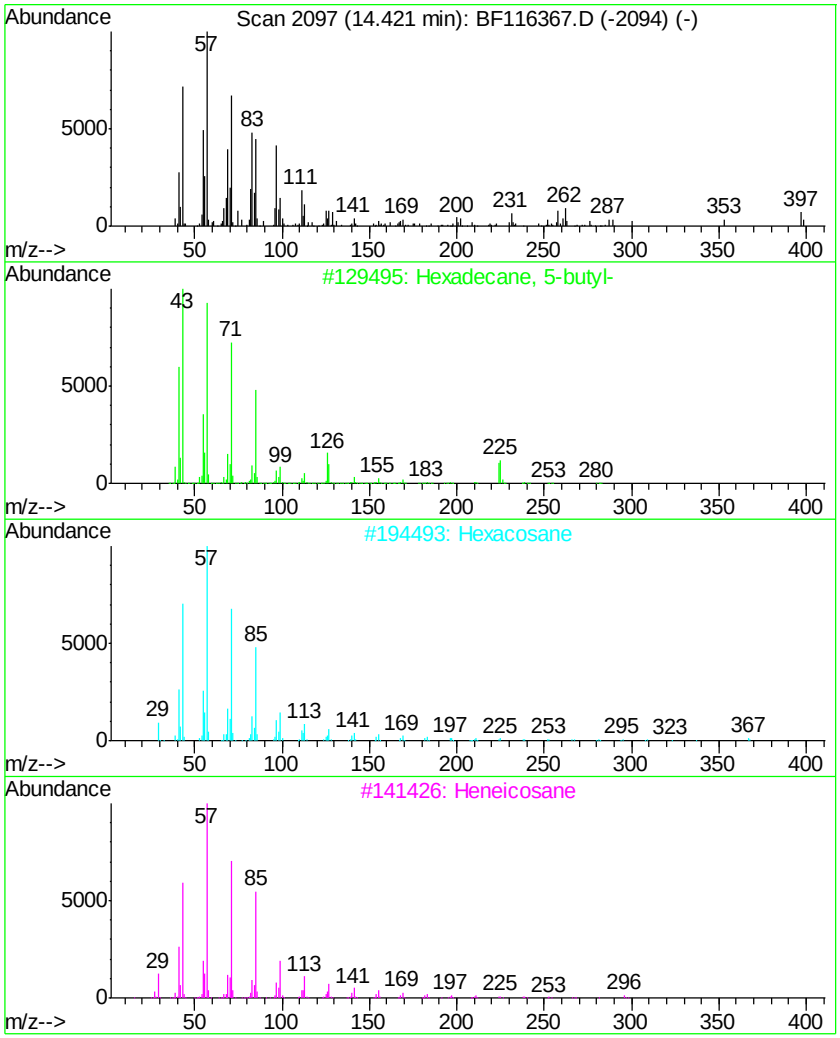
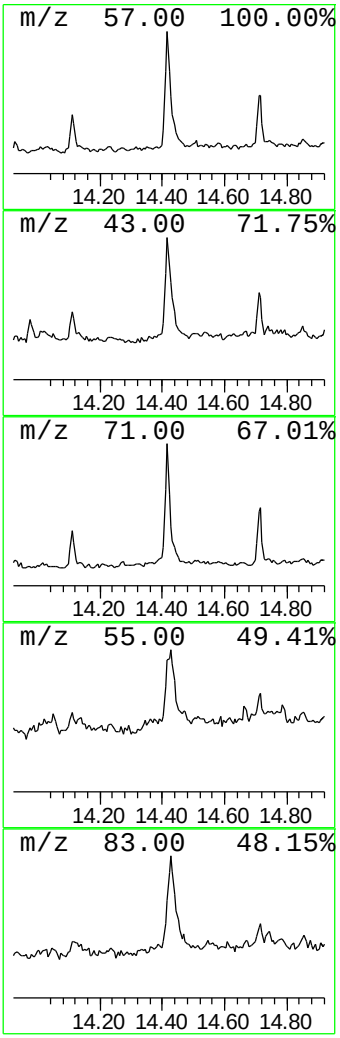
Peak Number 9 Hexadecane, 5-butyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	3.65 ng	179005	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





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Acq On : 17 Aug 2019 19:40
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Sample : K4223-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-10

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

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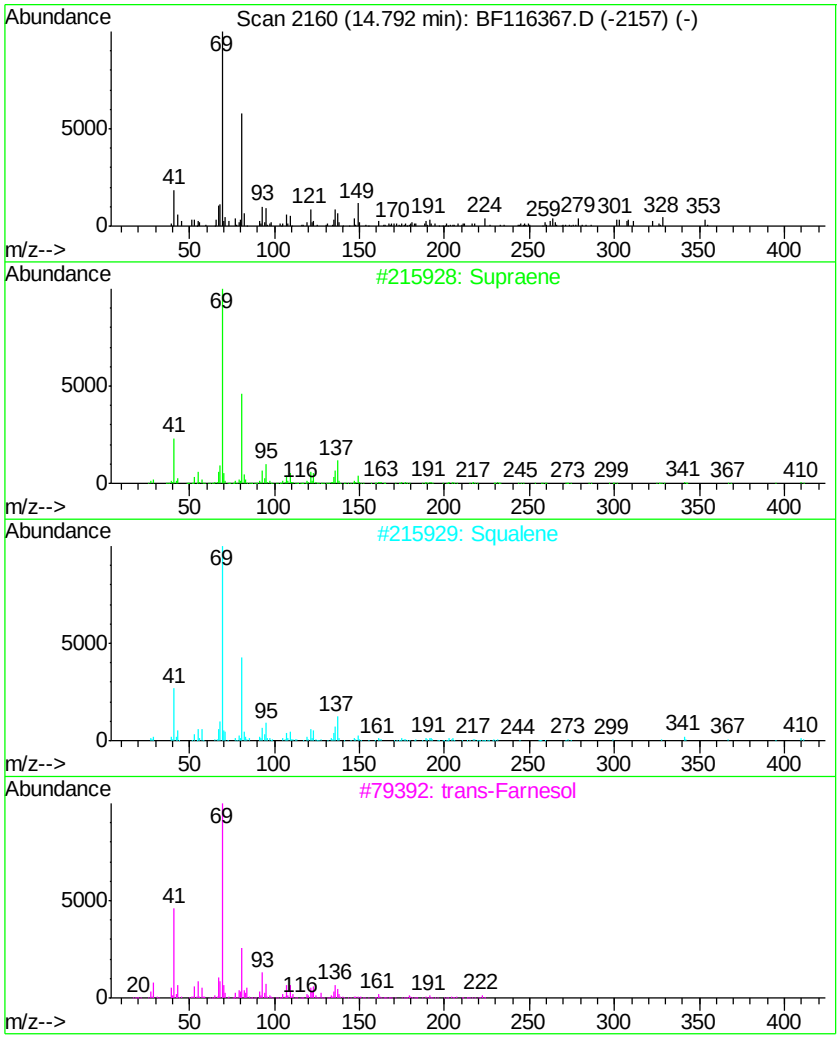
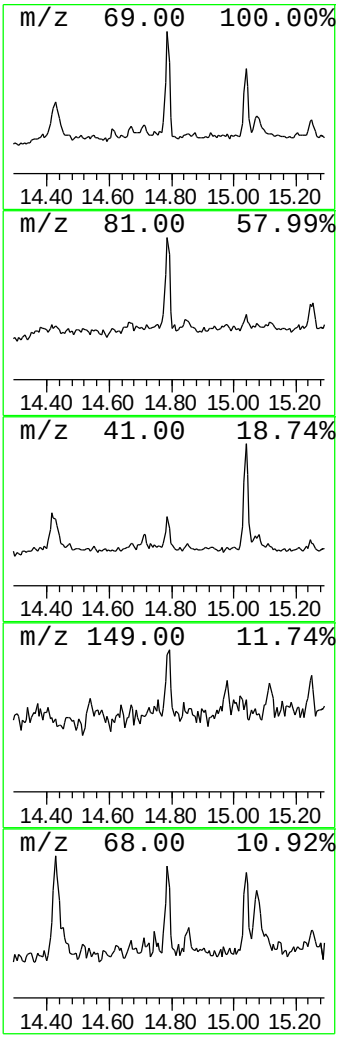
Peak Number 10 Squalene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.16 ng	77011	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	72
3	trans-Farnesol	222	C15H26O	000106-28-5	64
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59
5	2,6-Octadiene, 1-(2-bromophenoxy...	308	C16H21BrO	1000163-04-5	59





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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-10

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

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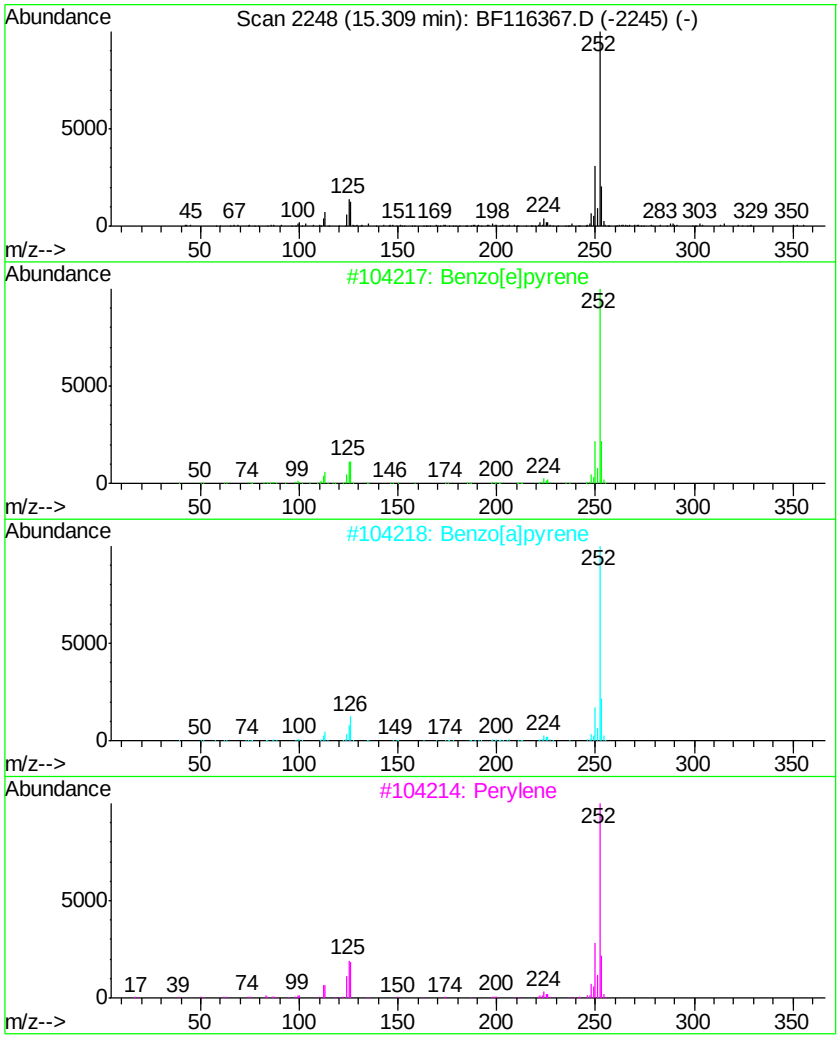
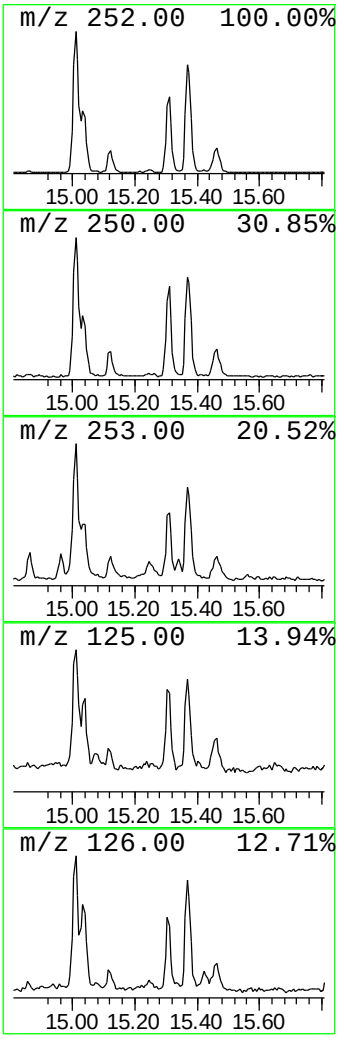
Peak Number 11 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.73 ng	97534	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Perylene	252	C20H12	000198-55-0	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





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Operator : HP/JU
Sample : K4223-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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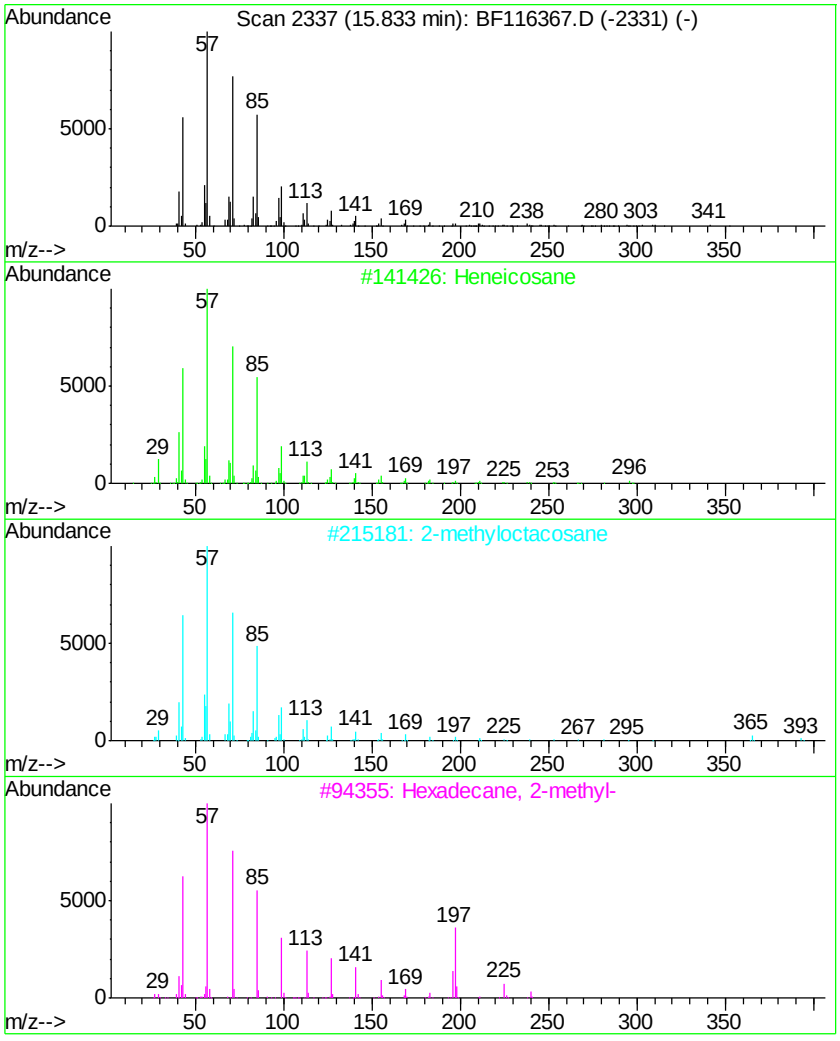
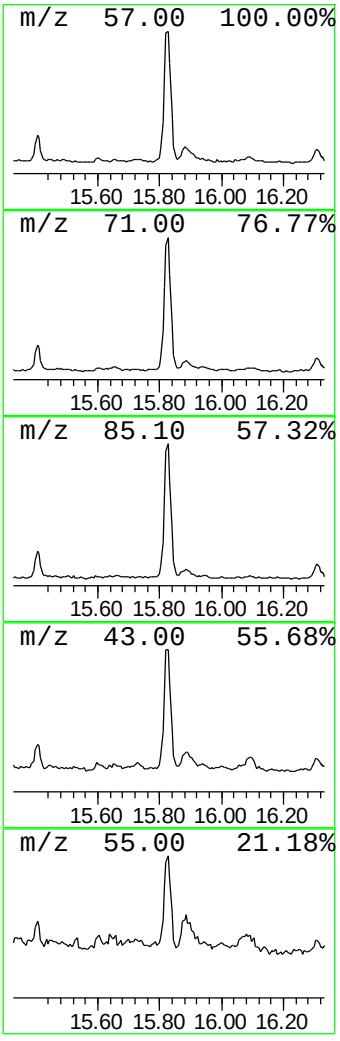
Peak Number 12 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	11.64 ng	415829	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87





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Sample : K4223-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
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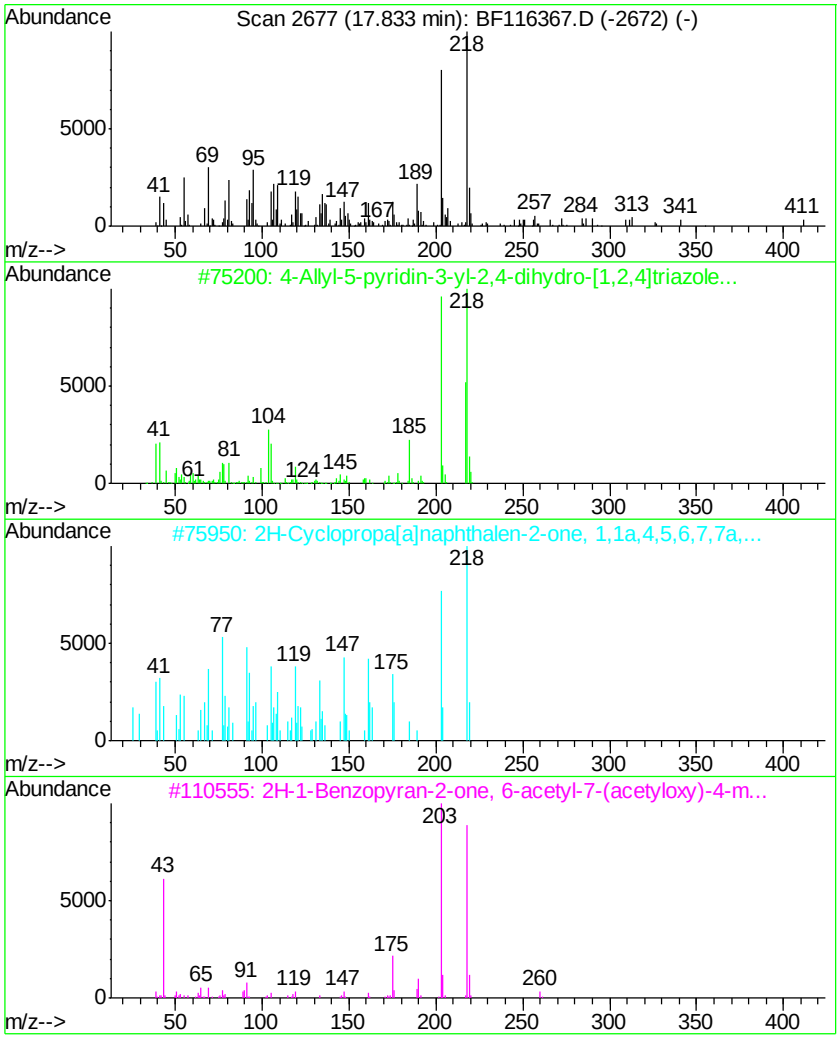
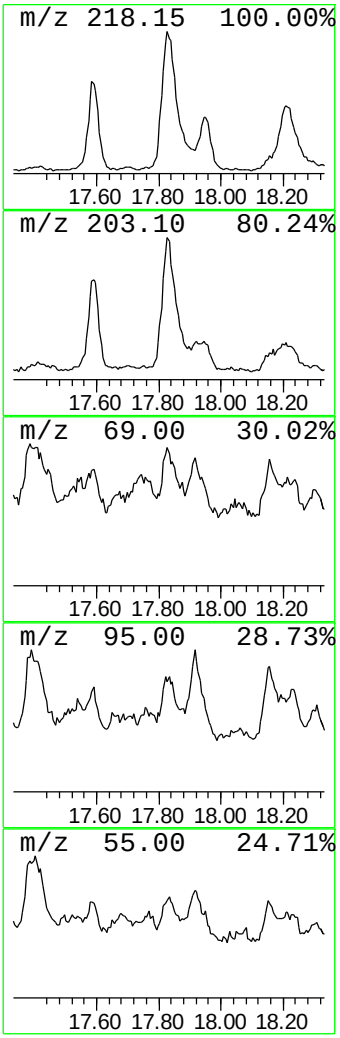
Peak Number 13 4-Allyl-5-pyridin-3-yl-2,4-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	7.32 ng	261334	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Allyl-5-pyridin-3-yl-2,4-dihyd...	218	C10H10N4S	1000300-40-5	58
2	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	58
3	2H-1-Benzopyran-2-one, 6-acetyl-...	260	C14H12O5	129812-31-3	50
4	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	50
5	Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	49





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Instrument : BNA_F
ClientSampleId : SP-10

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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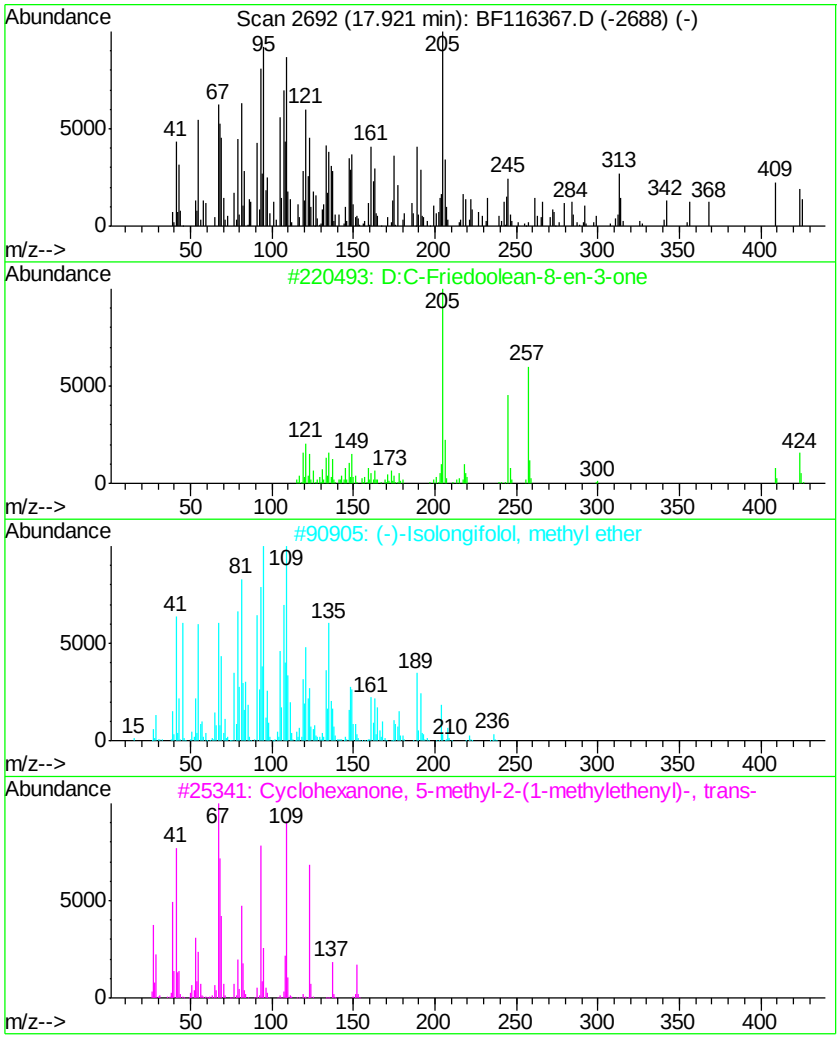
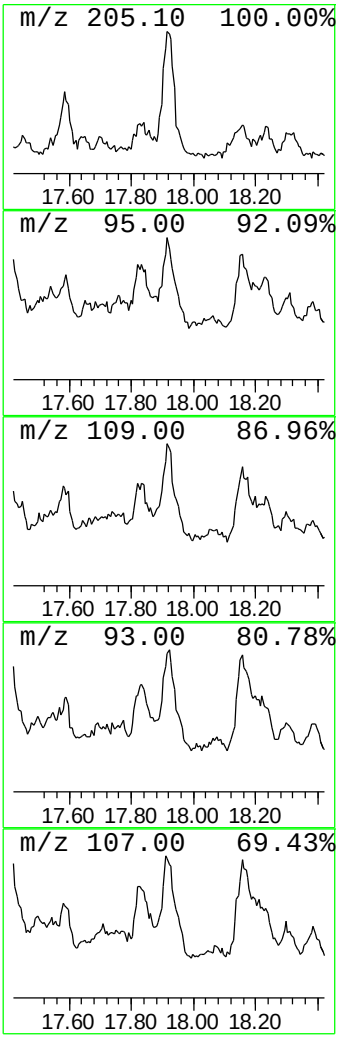
Peak Number 14 D:C-Friedoolean-8-en-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	12.34 ng	440686	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	70
2	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	43
3	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	029606-79-9	30
4	Furan-2-carboxamide, N-(2-fluoro...	205	C11H8FNO2	1000308-20-1	27
5	1,1-(Phenylthio)-2-isopropyl-cyc...	314	C19H22S2	122732-90-5	25





Library Search Compound Report

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

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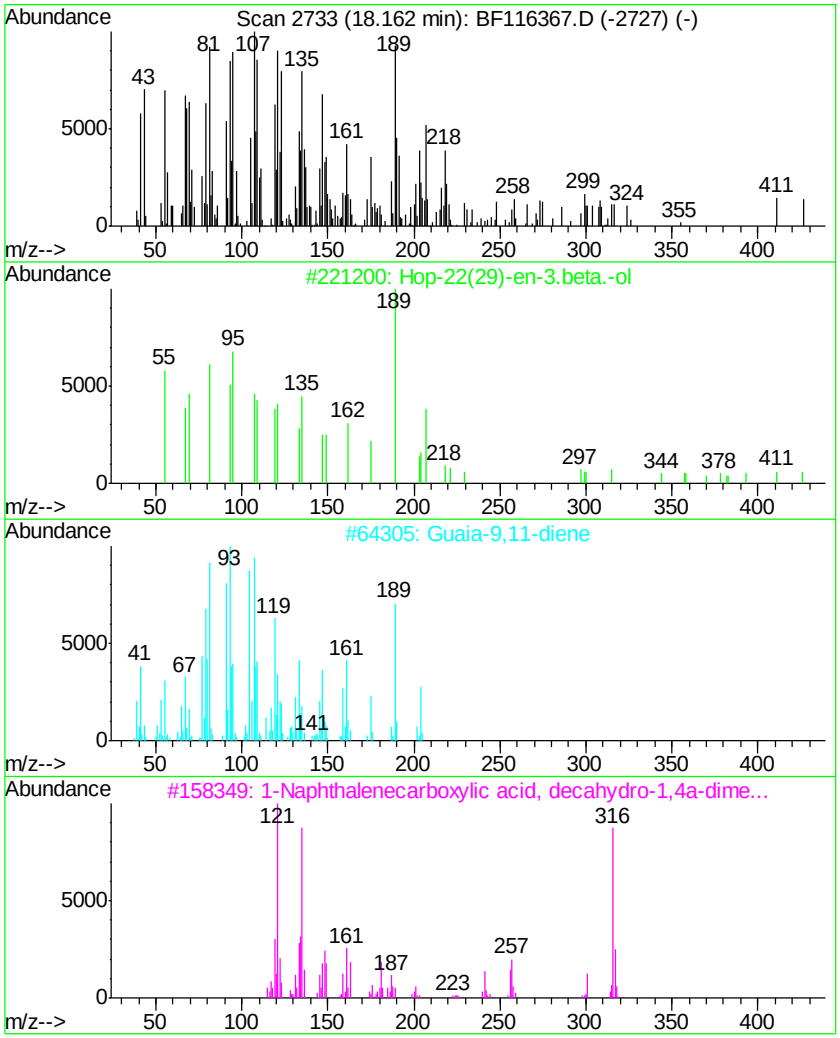
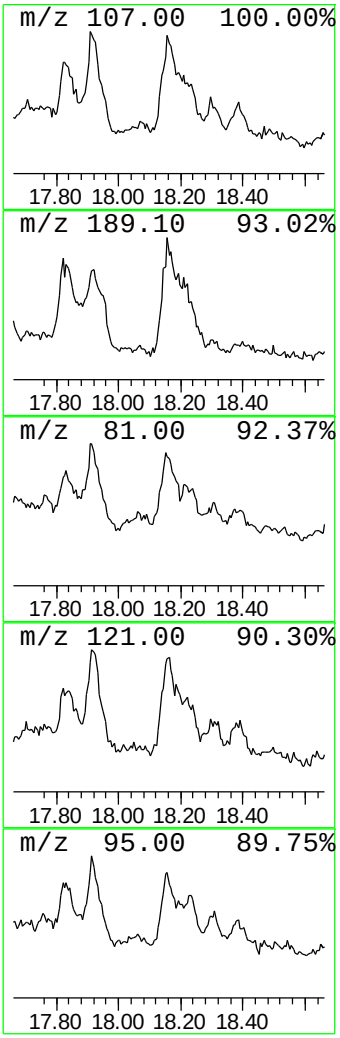
Peak Number 15 Hop-22(29)-en-3.beta.-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	7.19 ng	256858	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	64
2	Guaia-9,11-diene	204	C15H24	1000374-19-8	53
3	1-Naphthalenecarboxylic acid, de...	316	C21H32O2	001235-39-8	46
4	7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	41
5	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	38





Tentatively Identified Compound (LSC) summary

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Data File : BF116367.D
Acq On : 17 Aug 2019 19:40
Operator : HP/JU
Sample : K4223-19
Misc :
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ClientSampleId : SP-10

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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
unknown6.59	6.59	69.6	ng	2967850	1	6.81	853096	20.0
Palmitoleic acid	11.78	5.0	ng	279975	4	11.33	1118370	20.0
n-Hexadecanoic acid	11.86	12.4	ng	695434	4	11.33	1118370	20.0
Octadecanoic acid	12.63	3.3	ng	183026	4	11.33	1118370	20.0
Phenanthrene, 2,3...	12.83	2.6	ng	125830	5	13.97	981002	20.0
2-Phenanthrenol, ...	13.33	2.2	ng	109146	5	13.97	981002	20.0
Pentafluoropropio...	13.79	10.7	ng	527009	5	13.97	981002	20.0
Hexadecane, 5-butyl-	14.42	3.6	ng	179005	5	13.97	981002	20.0
Squalene	14.79	2.2	ng	77011	6	15.43	714427	20.0
Benzo[e]pyrene	15.31	2.7	ng	97534	6	15.43	714427	20.0
Heneicosane	15.83	11.6	ng	415829	6	15.43	714427	20.0
4-Allyl-5-pyridin...	17.83	7.3	ng	261334	6	15.43	714427	20.0
D:C-Friedoolean-8...	17.92	12.3	ng	440686	6	15.43	714427	20.0
Hop-22(29)-en-3.b...	18.16	7.2	ng	256858	6	15.43	714427	20.0