LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

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-BF122419.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	5.051	500	504	515	rBV	238369	294231	12.08%	1.349%
2	5.463	571	574	600	rBV	1590600	1731771	71.11%	7.940%
3	6.486	744	748	766	rBV	1965324	1863358	76.52%	8.543%
4	6.616	766	770	774	rBV	2105927	1997416	82.02%	9.158%
5	6.845	806	809	818	rBV	613519	492538	20.23%	2.258%
6	7.004	832	836	839	rBV	1643584	1500644	61.62%	6.880%
7	7.410	901	905	920	rBV	1061380	1133906	46.56%	5.199%
8	8.133	1024	1028	1043	rBV	703734	682238	28.02%	3.128%
9	9.210	1207	1211	1214	rBV	3033011	2435175	100.00%	11.165%
10	9.610	1275	1279	1287	rVB	107822	106354	4.37%	0.488%
11	9.892	1323	1327	1332	rBV	908045	772824	31.74%	3.543%
12	10.686	1458	1462	1477	rBV	1288567	1329067	54.58%	6.094%
13	11.386	1577	1581	1584	rBV	792231	733028	30.10%	3.361%
14	11.410	1584	1585	1591	rVB	132285	104025	4.27%	0.477%
15	11.910	1662	1670	1678	rBV3	161286	221278	9.09%	1.015%
16	12.610	1786	1789	1793	rBV	258258	232910	9.56%	1.068%
17	12.698	1802	1804	1810	rBV4	29907	37863	1.55%	0.174%
18	12.839	1823	1828	1834	rBV	226449	227862	9.36%	1.045%
19	12.974	1847	1851	1855	rBV	2202301	2062725	84.71%	9.457%
20	13.168	1877	1884	1886	rBV3	28716	40874	1.68%	0.187%
21	13.292	1903	1905	1910	rVB5	30357	35933	1.48%	0.165%
22	13.404	1921	1924	1927	rBV3	52513	56592	2.32%	0.259%
23	13.439	1927	1930	1936	rVB6	46831	78936	3.24%	0.362%
24	13.792	1987	1990	1993	rBV	32140	36226	1.49%	0.166%
25	13.874	2000	2004	2014	rVB4	193947	358225	14.71%	1.642%
26	14.004	2023	2026	2028	rBV	61583	61655	2.53%	0.283%
27	14.045	2028	2033	2036	rVV2	661898	780085	32.03%	3.577%
28	14.068	2036	2037	2040	rVB	114638	72391	2.97%	0.332%
29	14.186	2054	2057	2059	rBV	69456	58809	2.41%	0.270%
30	14.433	2097	2099	2102	rVB	38303	31219	1.28%	0.143%
31	14.492	2106	2109	2111	rBV	126355	106301	4.37%	0.487%
32	14.798	2158	2161	2165	rVB	128413	121607	4.99%	0.558%
33	14.874	2171	2174	2177	rVB	44558	43798	1.80%	0.201%
34	14.945	2182	2186	2189	rBV4	35005	51190	2.10%	0.235%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.098	2208	2212	2215	rBV	113840	166119	6.82%	0.762%
36	15.139	2216	2219	2223	rVB	153625	180838	7.43%	0.829%
37	15.204	2228	2230	2236	rVB3	40759	59339	2.44%	0.272%
38	15.351	2251	2255	2256	rBV4	24263	29402	1.21%	0.135%
39	15.404	2261	2264	2271	rVV2	81233	143336	5.89%	0.657%
40	15.468	2272	2275	2279	rVB	87300	113143	4.65%	0.519%
41	15.527	2280	2285	2295	rVV2	453955	694458	28.52%	3.184%
42	15.962	2355	2359	2364	rBV	102528	171095	7.03%	0.784%
43	16.051	2368	2374	2381	rBV	44720	130569	5.36%	0.599%
44	16.474	2442	2446	2449	rVB2	41213	67575	2.77%	0.310%
45	17.045	2540	2543	2544	rBV2	43308	46310	1.90%	0.212%
46	17.203	2565	2570	2572	rBV6	27804	44450	1.83%	0.204%
47	17.615	2635	2640	2645	rBV9	31465	70887	2.91%	0.325%

Sum of corrected areas: 21810575

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
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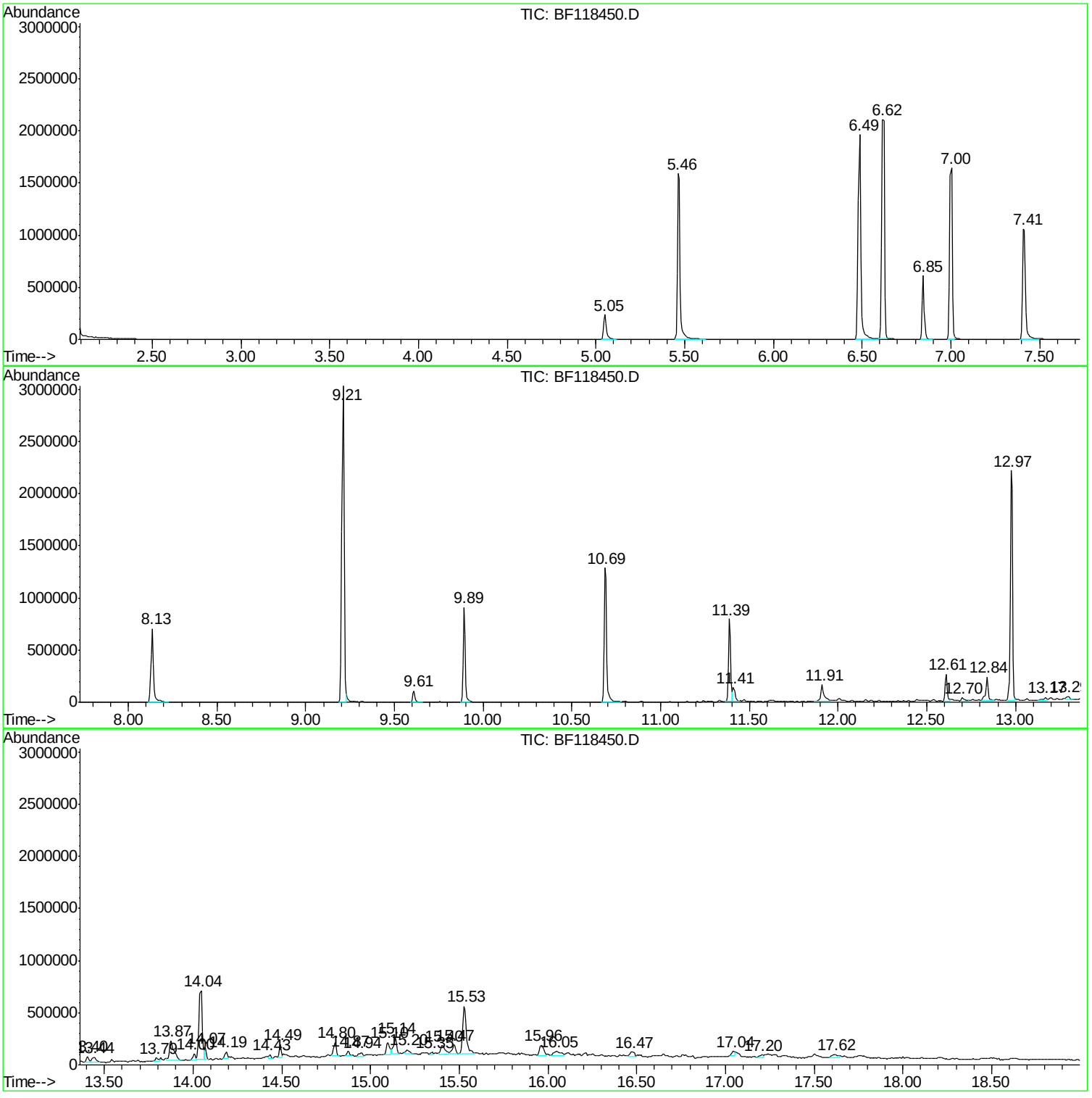
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

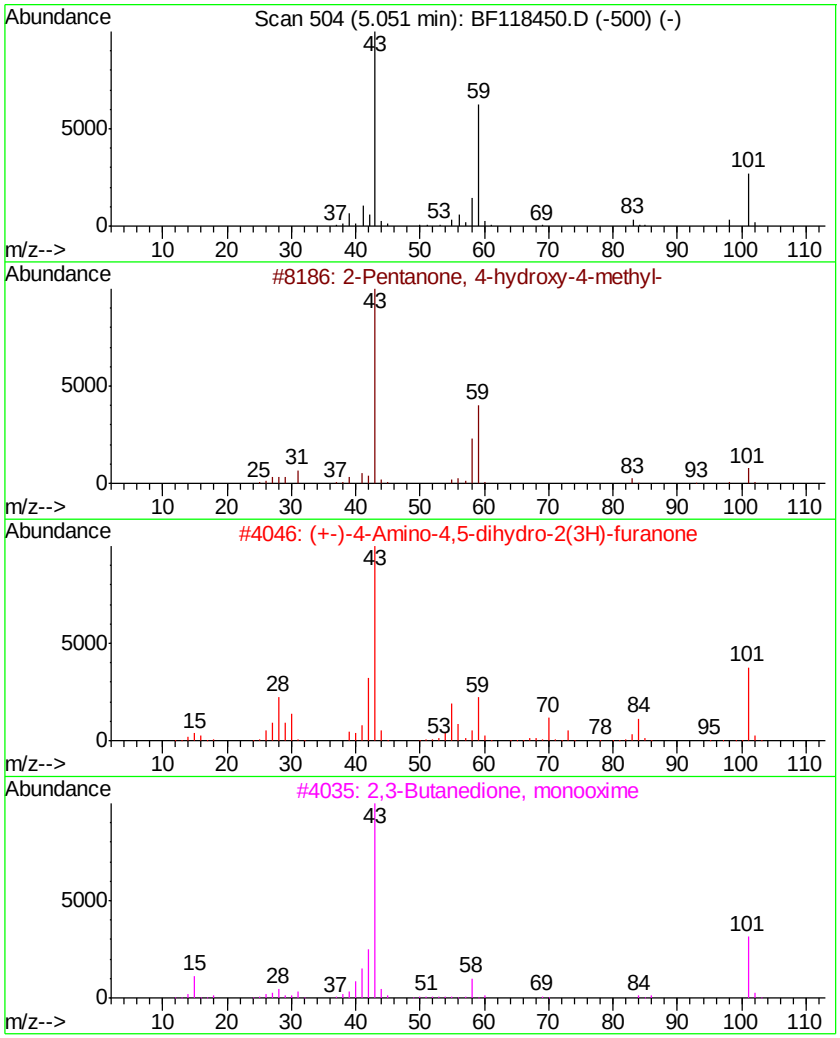
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

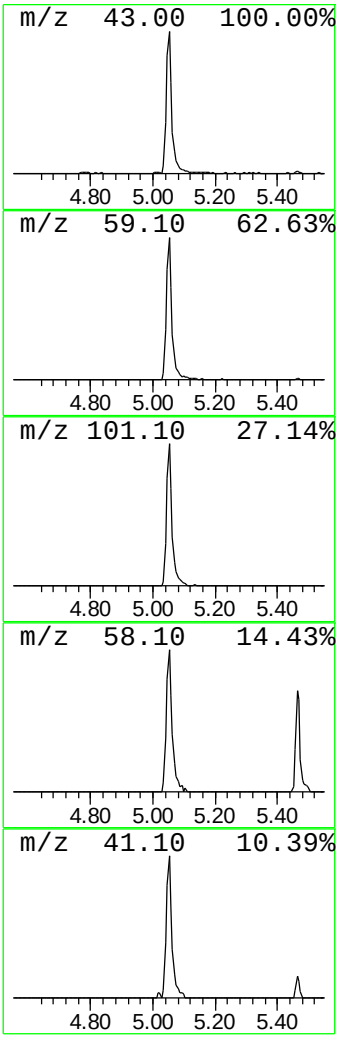
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	11.95 ng	294231	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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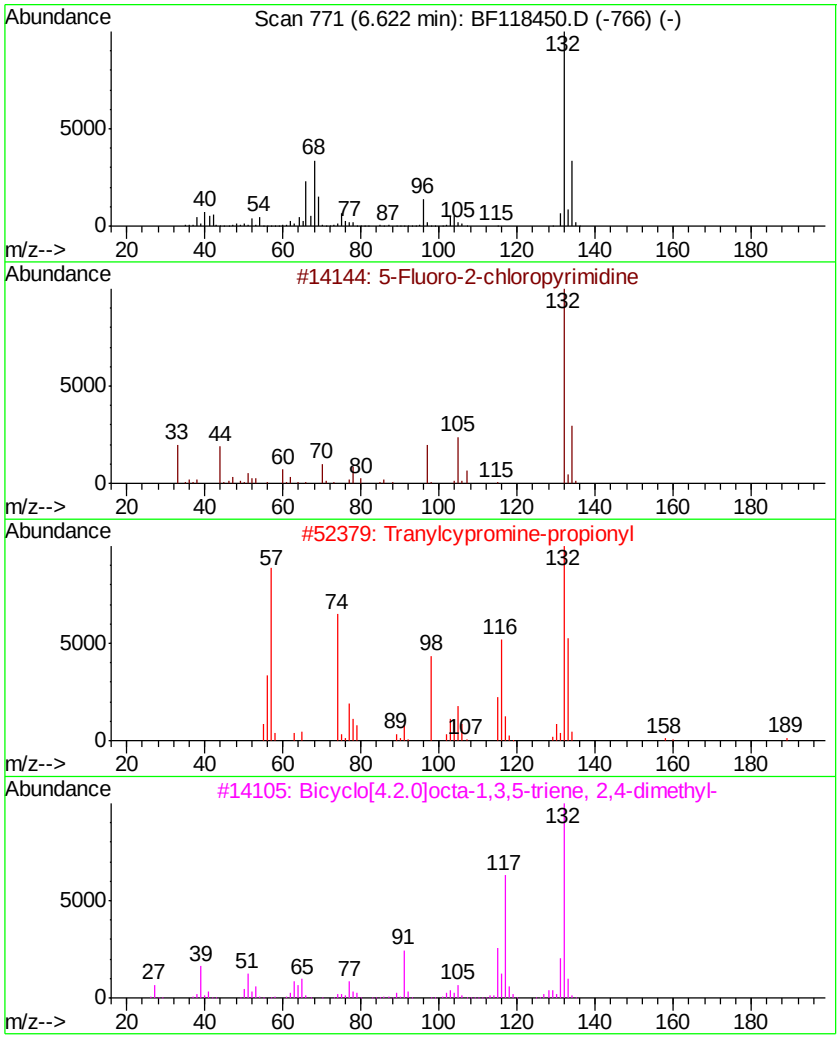
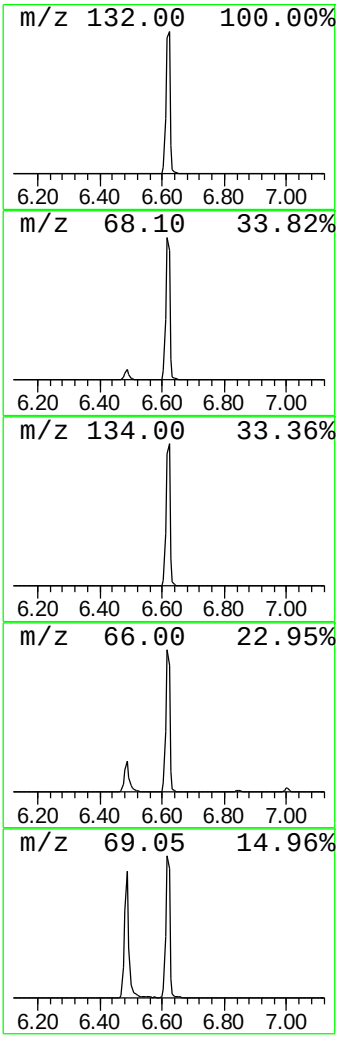
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	81.11 ng	1997420	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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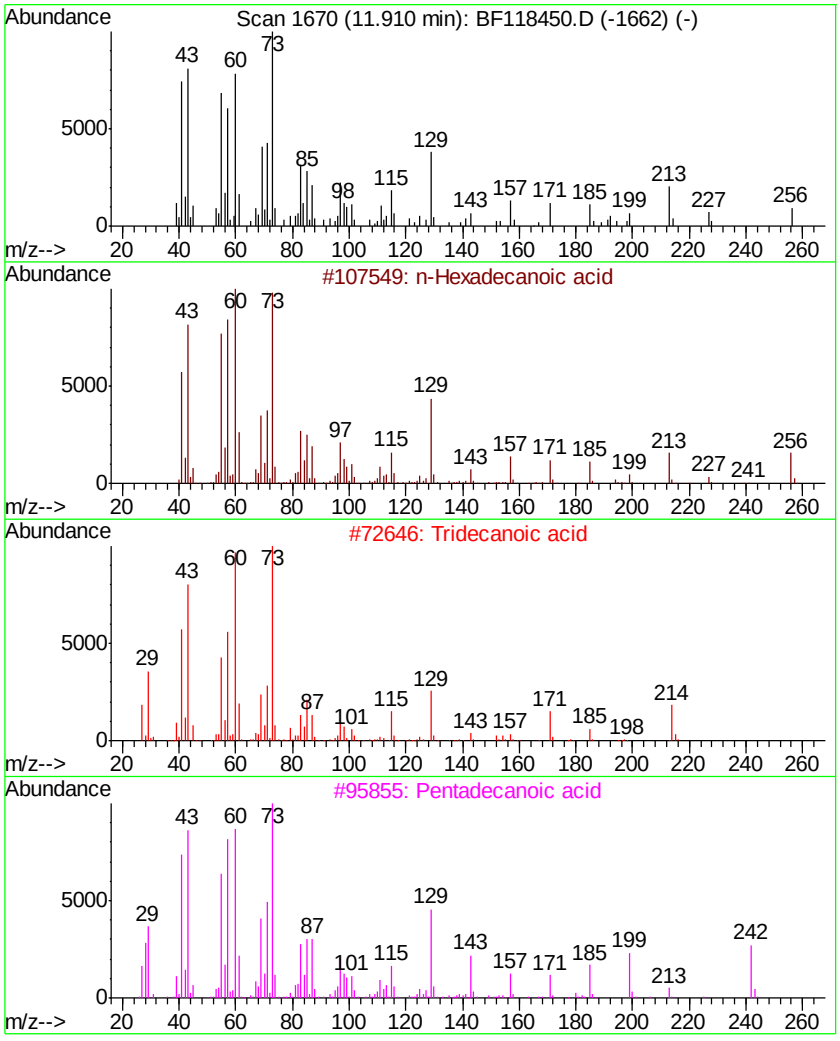
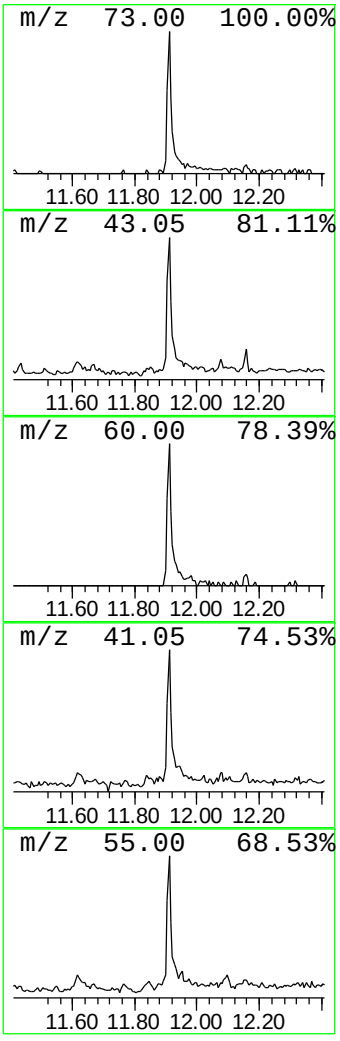
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	6.04 ng	221278	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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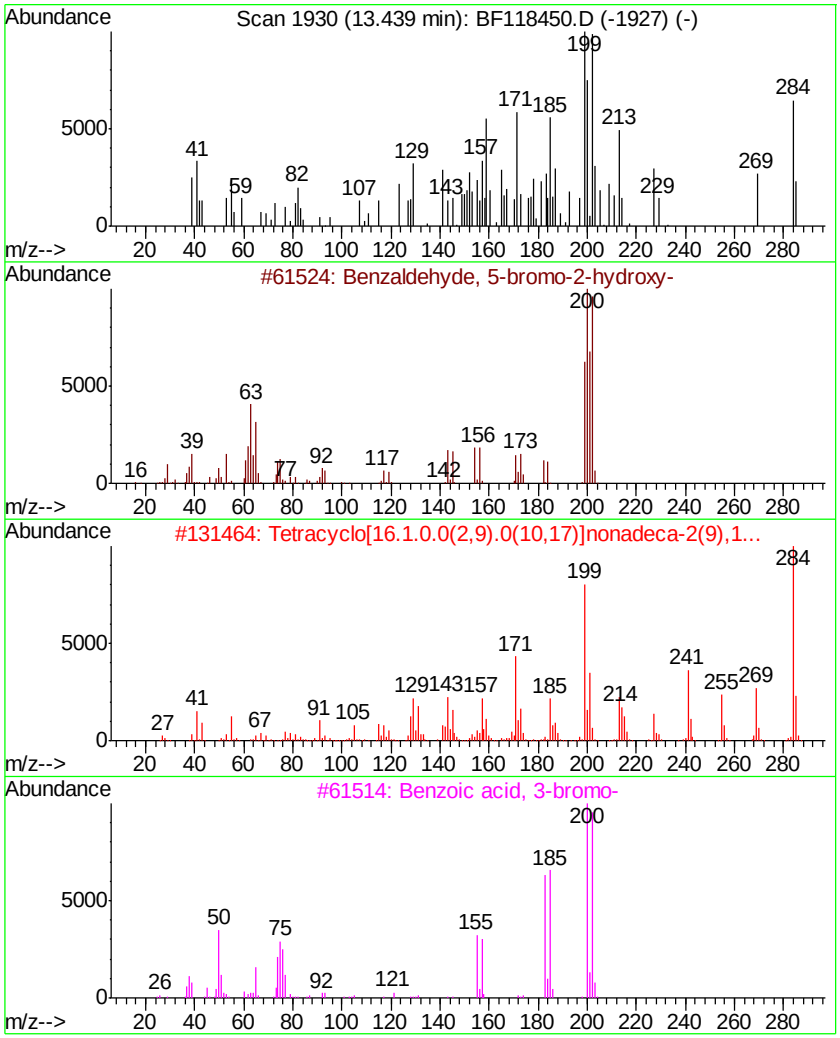
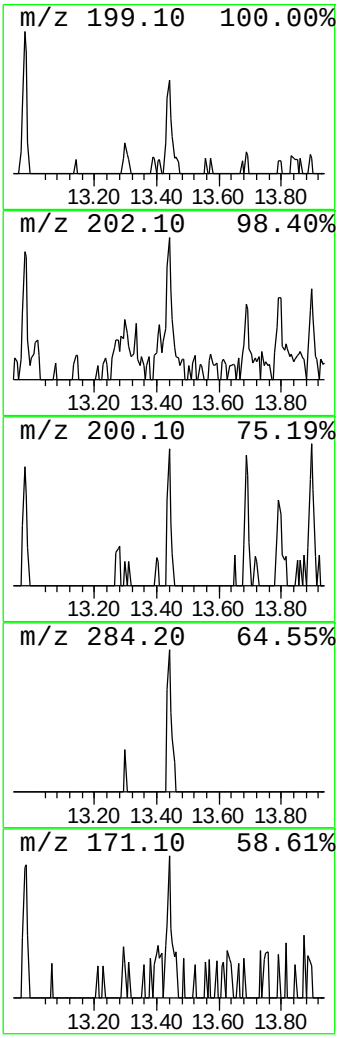
Peak Number 5 unknown13.44 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.02 ng	78936	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 5-bromo-2-hydroxy-	200	C7H5BrO2	001761-61-1	38
2	Tetracyclo[16.1.0.0(2,9).0(10,17...	284	C21H32	1000163-57-5	35
3	Benzoic acid, 3-bromo-	200	C7H5BrO2	000585-76-2	27
4	5-Bromophthaldehydic acid	228	C8H5BrO3	004785-52-8	25
5	Estra-1,3,5(10)-trien-17-one, 3-...	284	C19H24O2	001624-62-0	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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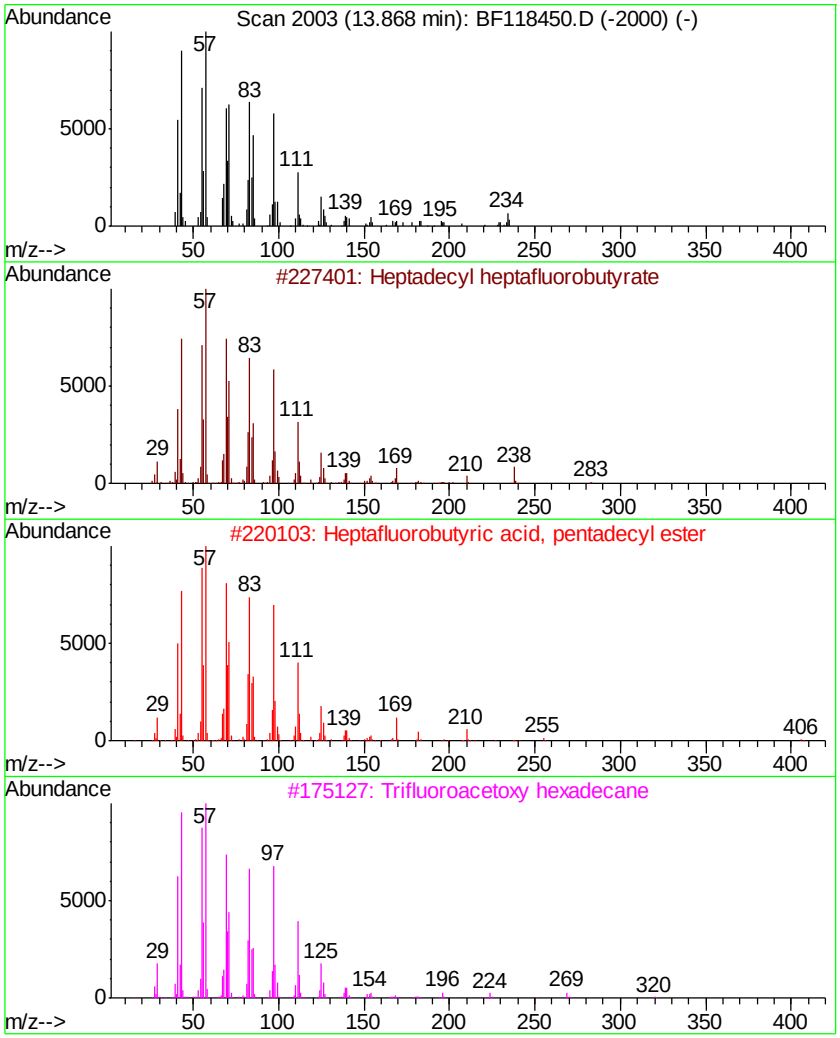
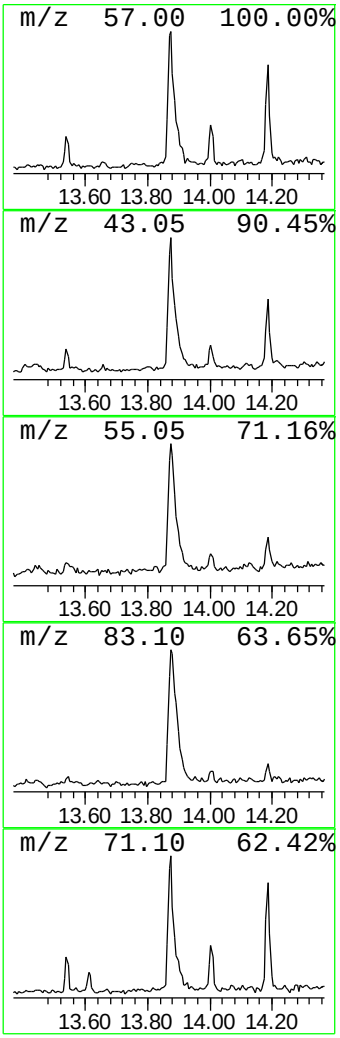
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.18 ng	358225	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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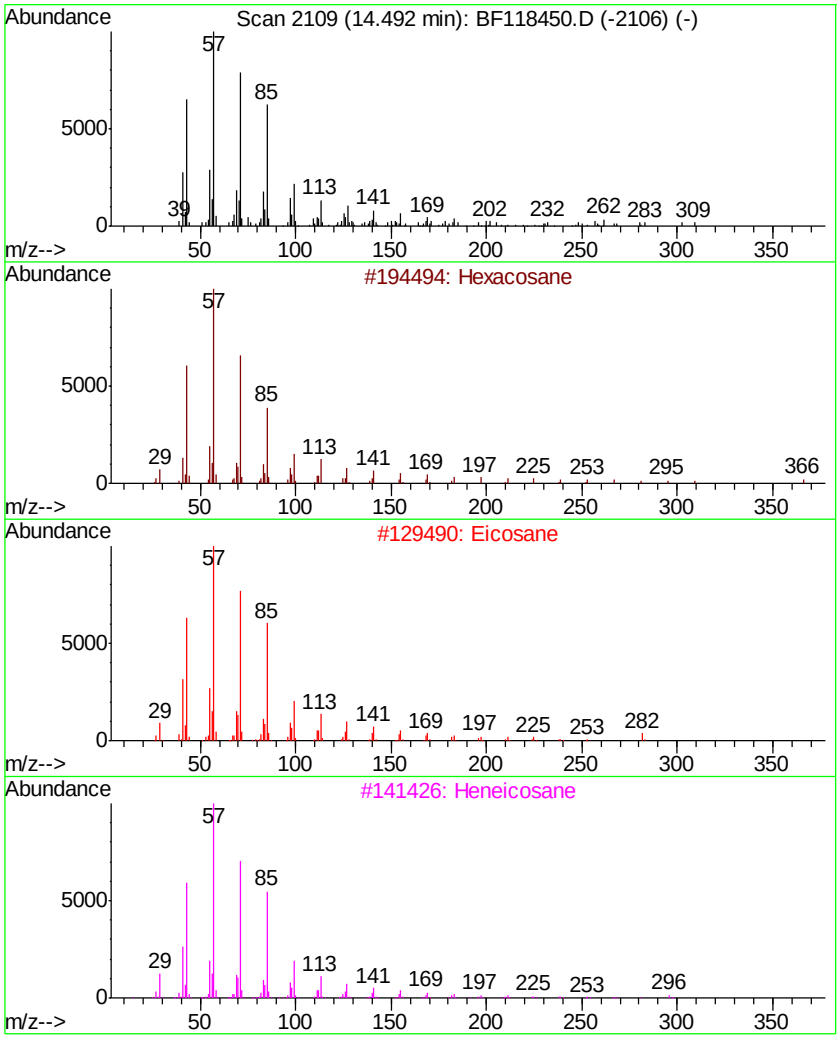
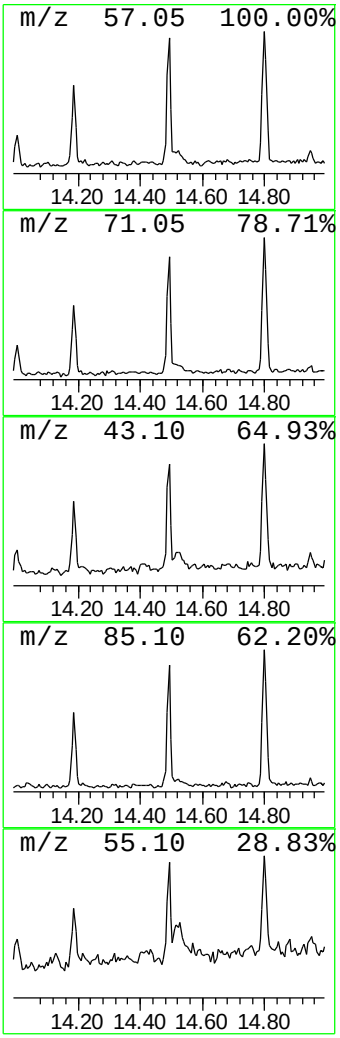
Peak Number 7 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.73 ng	106301	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Nonadecane	268	C19H40	000629-92-5	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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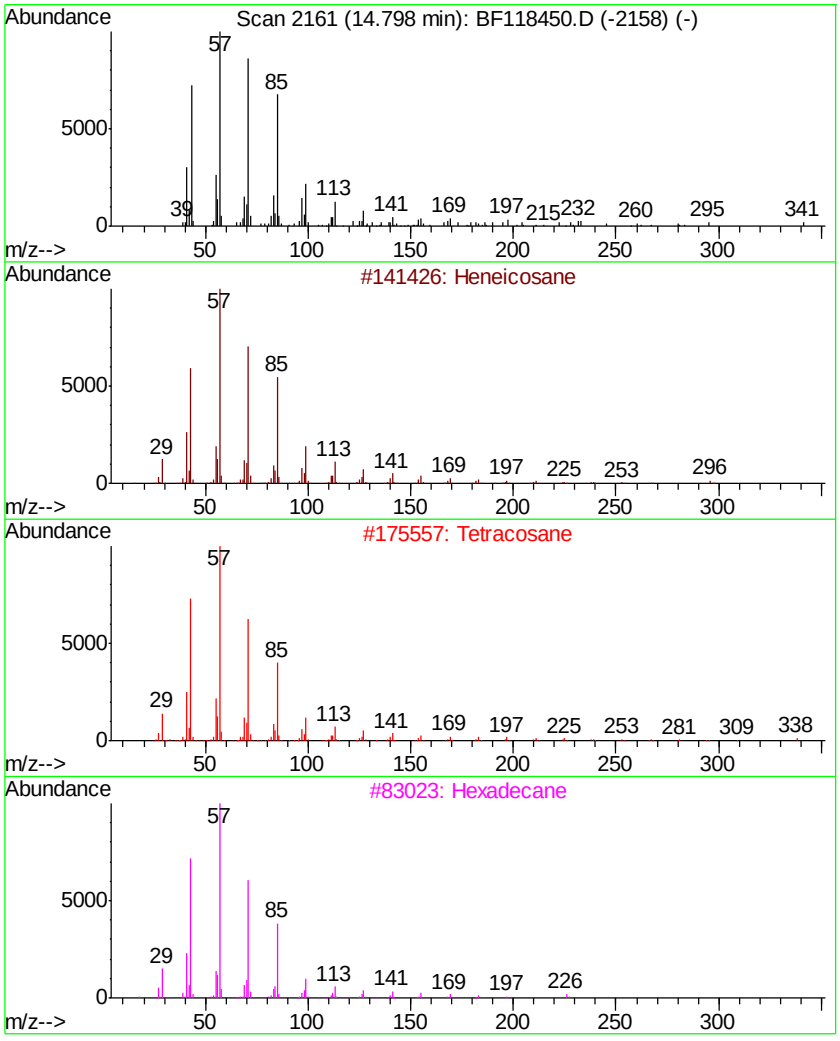
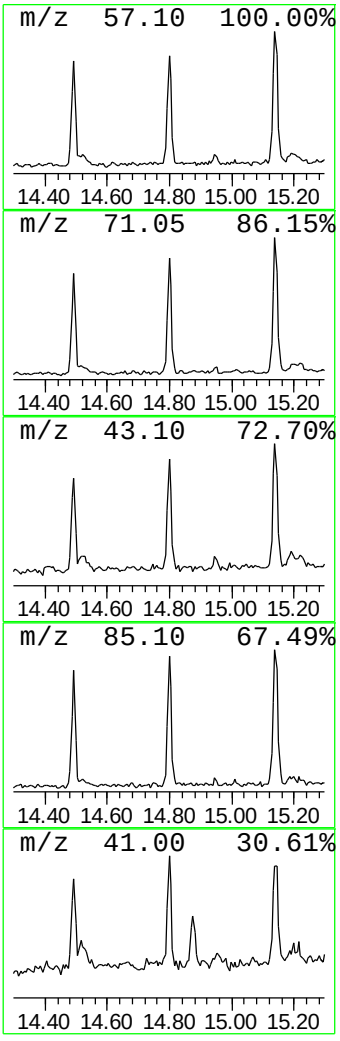
Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.50 ng	121607	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	80
3	Hexadecane	226	C16H34	000544-76-3	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Nonadecane	268	C19H40	000629-92-5	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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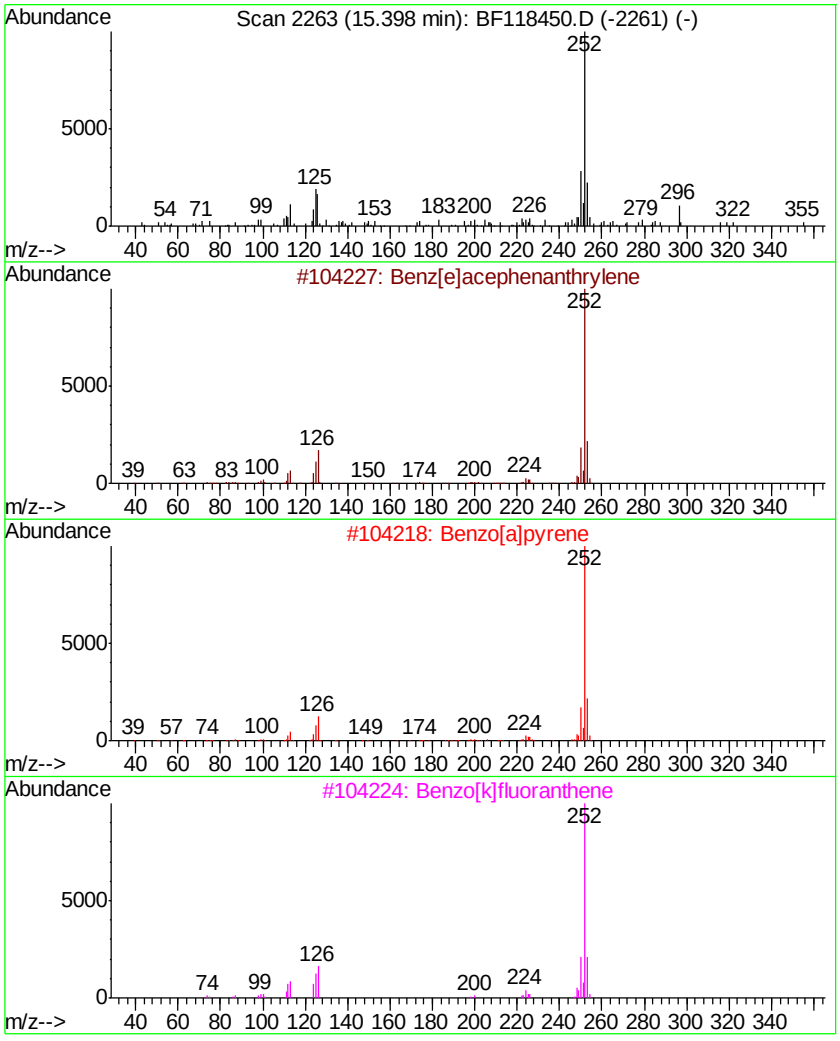
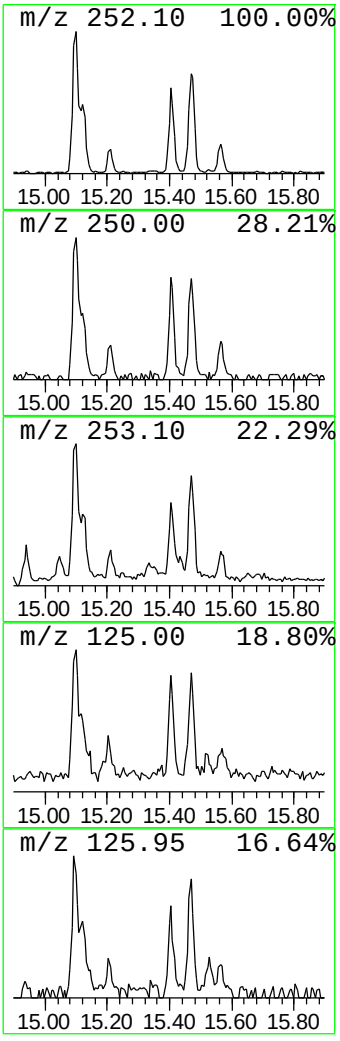
Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	4.13 ng	143336	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[e]pyrene	252	C20H12	000192-97-2	95
5	Perylene	252	C20H12	000198-55-0	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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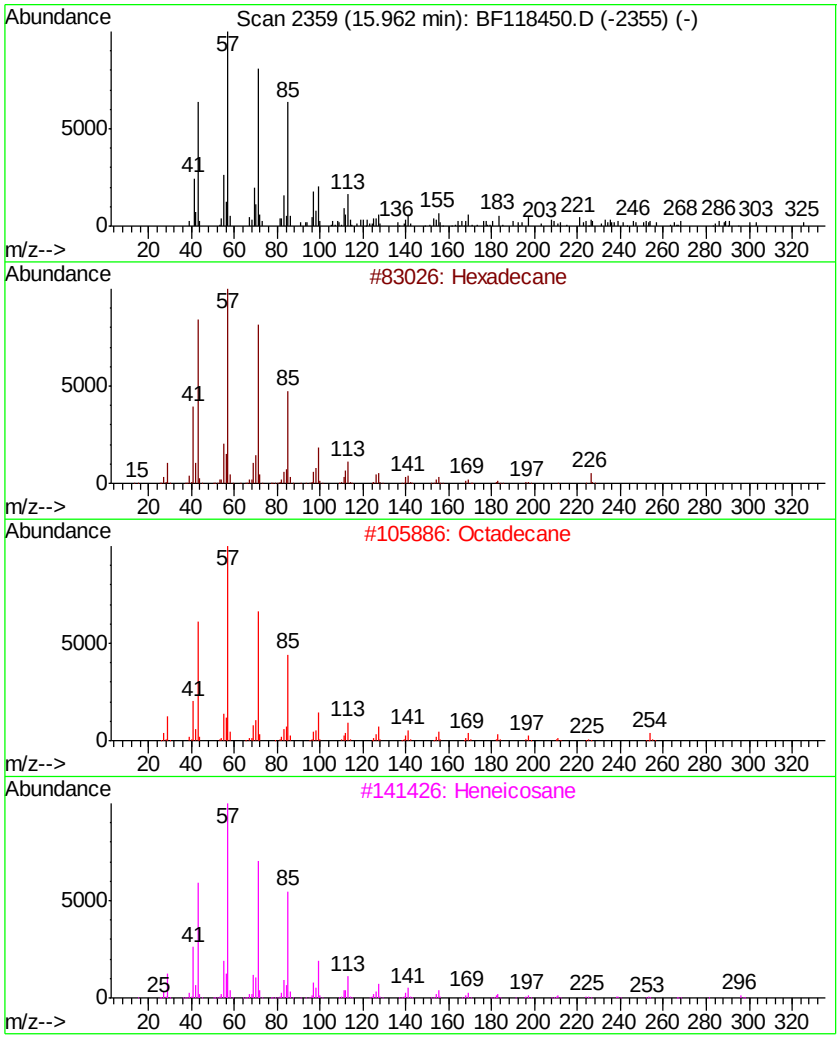
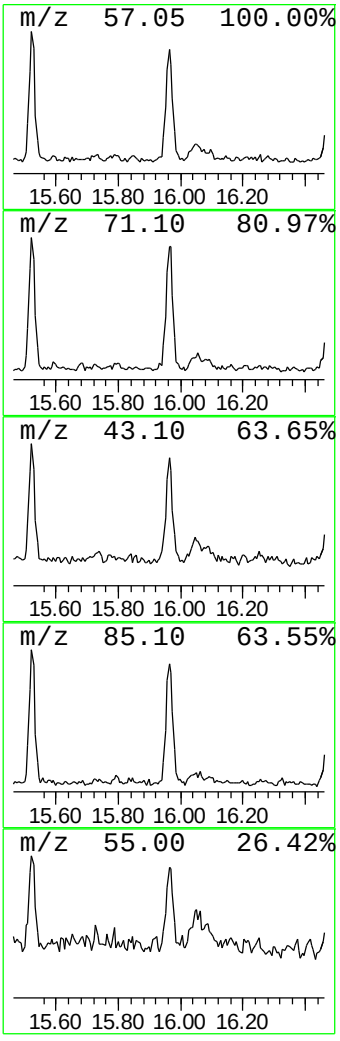
Peak Number 10 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	4.93 ng	171095	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Octadecane	254	C18H38	000593-45-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Pentadecane	212	C15H32	000629-62-9	87
5	Nonadecane	268	C19H40	000629-92-5	87





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Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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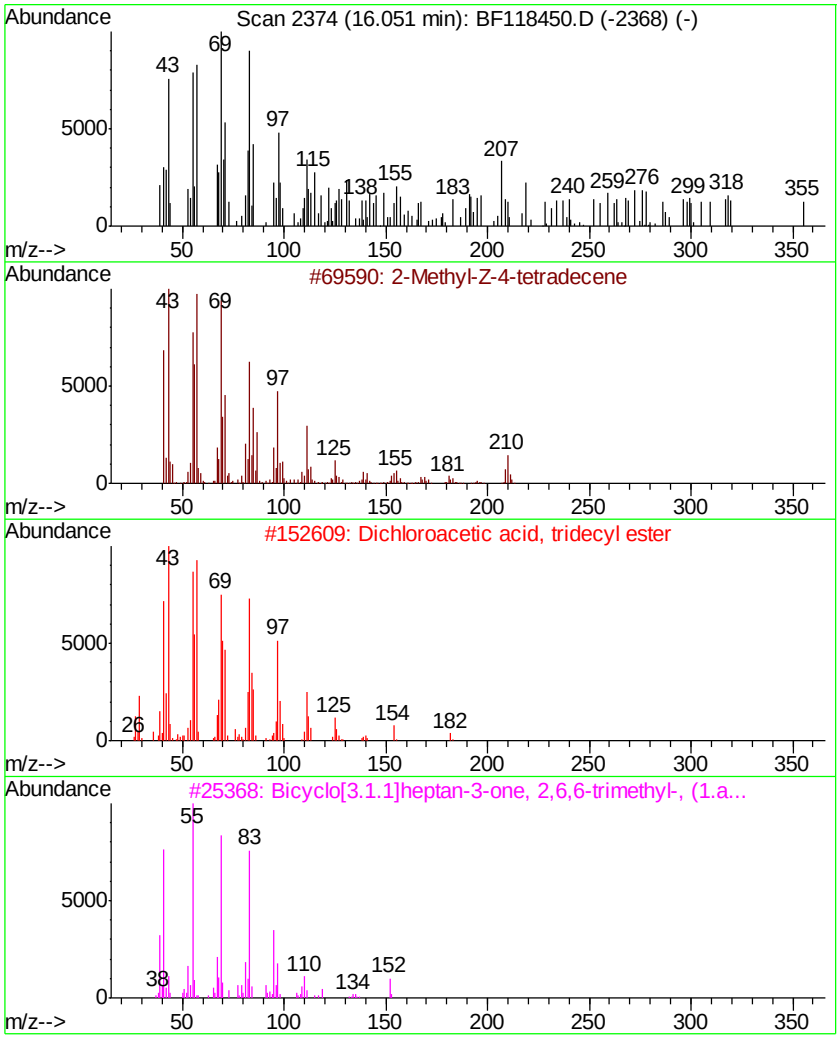
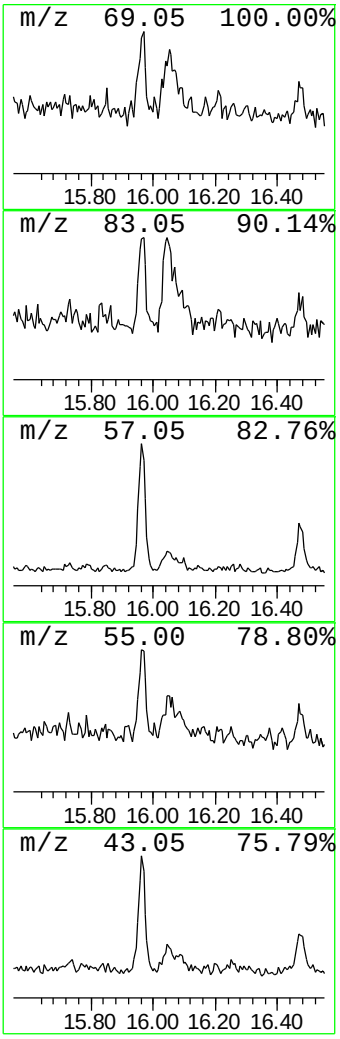
Peak Number 11 2-Methyl-Z-4-tetradecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	3.76 ng	130569	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	83
2	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	62
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	53
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	43
5	Cyclopentanone, 3-(3-hydroxy-1-p...	140	C8H12O2	074473-08-8	42





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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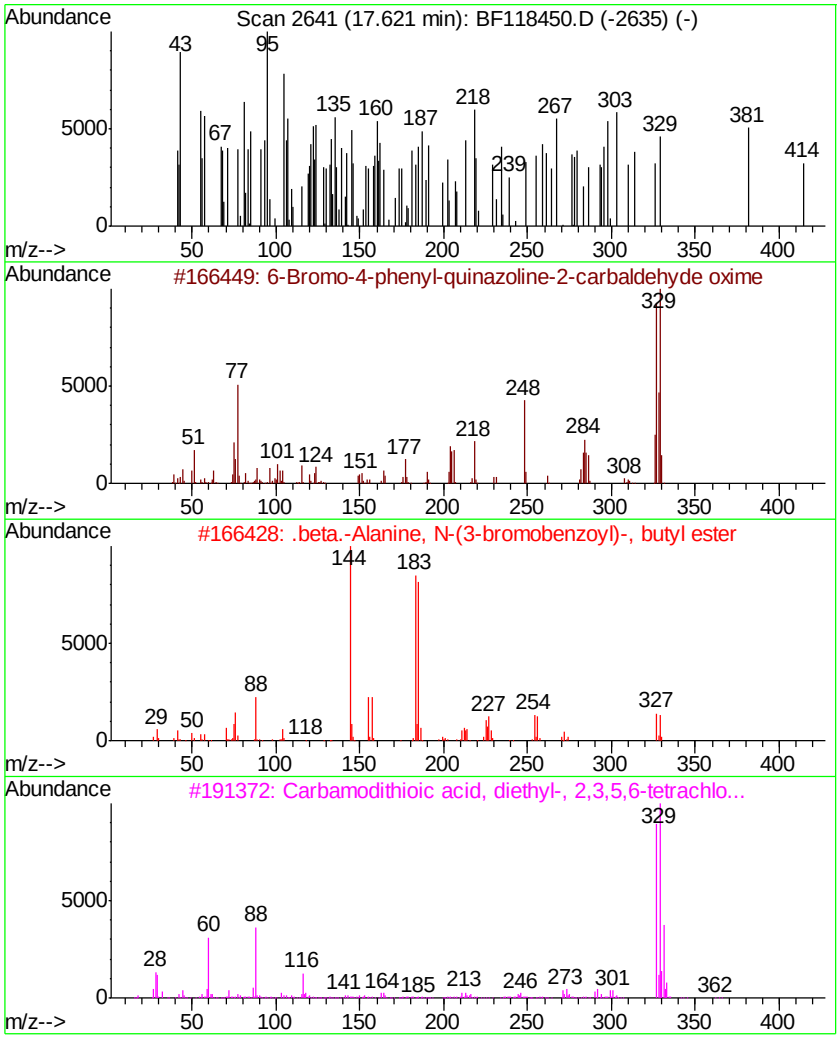
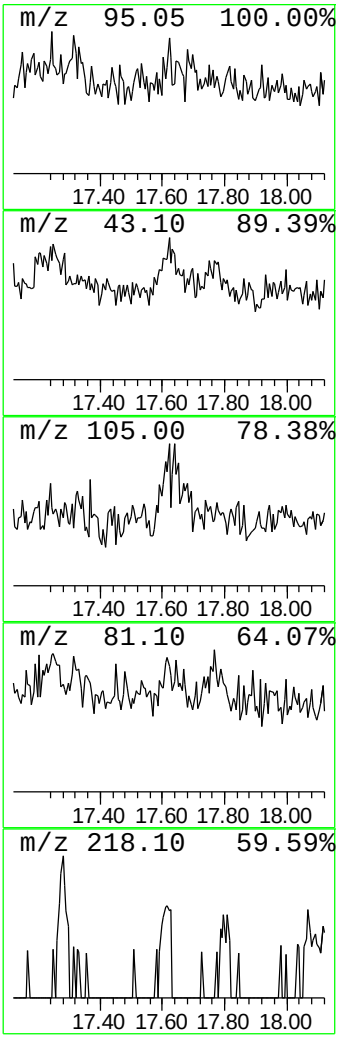
Peak Number 12 unknown17.62 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	2.04 ng	70887	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Bromo-4-phenyl-quinazoline-2-c...	327	C15H10BrN3O	1000317-60-7	9
2	.beta.-Alanine, N-(3-bromobenzoy...	327	C14H18BrNO3	1000321-64-0	9
3	Carbamodithioic acid, diethyl-, ...	362	C10H10Cl4N2S2	1000305-30-3	9
4	3-Bromo-7,9-dichloro-5-methylpyr...	327	C13H8BrCl2N	1000251-40-3	7
5	Salutaridinol	329	C19H23NO4	002392-98-5	7





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010220\
Data File : BF118450.D
Acq On : 2 Jan 2020 22:06
Operator : JU
Sample : K6465-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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
2-Pentanone, 4-hy...	5.05	11.9	ng	294231	1	6.85	492538	20.0
unknown6.62	6.62	81.1	ng	1997420	1	6.85	492538	20.0
n-Hexadecanoic acid	11.91	6.0	ng	221278	4	11.39	733028	20.0
unknown13.44	13.44	2.0	ng	78936	5	14.04	780085	20.0
Heptadecyl heptaf...	13.87	9.2	ng	358225	5	14.04	780085	20.0
Hexacosane	14.49	2.7	ng	106301	5	14.04	780085	20.0
Heneicosane	14.80	3.5	ng	121607	6	15.53	694458	20.0
Benzo[e]pyrene	15.40	4.1	ng	143336	6	15.53	694458	20.0
Hexadecane	15.96	4.9	ng	171095	6	15.53	694458	20.0
2-Methyl-Z-4-tetr...	16.05	3.8	ng	130569	6	15.53	694458	20.0
unknown17.62	17.62	2.0	ng	70887	6	15.53	694458	20.0