LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\
Data File : BF107462.D
Acq On : 17 Jul 2018 21:01
Operator : JU/SJ
Sample : J3906-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-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-BF071618.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	3.619	214	218	225	rBV2	29971	48866	1.12%	0.103%
2	5.231	487	492	499	rBV	379952	502951	11.55%	1.064%
3	5.619	552	558	561	rBV	3885506	3943086	90.54%	8.342%
4	6.619	721	728	736	rBV	3569086	4355188	100.00%	9.214%
5	6.760	746	752	755	rBV	4152613	4170286	95.75%	8.823%
6	6.801	757	759	764	rVB	167836	132536	3.04%	0.280%
7	6.984	783	790	794	rVB	1157644	977753	22.45%	2.069%
8	7.143	813	817	820	rBV	3365652	3003997	68.98%	6.355%
9	7.548	877	886	889	rBV	2644444	2731760	62.72%	5.779%
10	8.266	1004	1008	1011	rBV	1249807	1132333	26.00%	2.396%
11	8.289	1011	1012	1015	rVB	226896	116065	2.66%	0.246%
12	8.984	1123	1130	1133	rBV	74476	74593	1.71%	0.158%
13	9.342	1186	1191	1194	rBV	4311889	4233971	97.22%	8.957%
14	9.448	1205	1209	1213	rVB	1609018	1598245	36.70%	3.381%
15	9.731	1254	1257	1261	rVB	824803	688562	15.81%	1.457%
16	10.031	1304	1308	1311	rBV	1257754	1155093	26.52%	2.444%
17	10.060	1311	1313	1316	rVB	186958	143029	3.28%	0.303%
18	10.231	1339	1342	1346	rVB	141146	124715	2.86%	0.264%
19	10.578	1397	1401	1402	rBV	204128	199549	4.58%	0.422%
20	10.595	1402	1404	1407	rVB	546508	417317	9.58%	0.883%
21	10.825	1438	1443	1446	rBV	2507147	2618524	60.12%	5.540%
22	11.419	1541	1544	1547	rVB	68513	60872	1.40%	0.129%
23	11.525	1558	1562	1564	rBV	1208792	1229397	28.23%	2.601%
24	11.548	1564	1566	1569	rVB	1123607	844740	19.40%	1.787%
25	11.595	1569	1574	1577	rBV	312442	287131	6.59%	0.607%
26	11.683	1585	1589	1591	rBV3	62729	62554	1.44%	0.132%
27	11.748	1594	1600	1605	rVB2	154981	175117	4.02%	0.370%
28	12.025	1640	1647	1649	rBV	100281	116069	2.67%	0.246%
29	12.048	1649	1651	1656	rVB2	137554	123229	2.83%	0.261%
30	12.101	1656	1660	1662	rVB3	60960	67082	1.54%	0.142%
31	12.136	1662	1666	1669	rBV3	172813	206096	4.73%	0.436%
32	12.319	1694	1697	1699	rBV	70848	63442	1.46%	0.134%
33	12.495	1725	1727	1733	rBV7	26368	43843	1.01%	0.093%
34	12.589	1741	1743	1752	rVB8	55323	110937	2.55%	0.235%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J3906-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-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-BF071618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.660	1752	1755	1759	rVB6	31590	46009	1.06%	0.097%
36	12.736	1764	1768	1773	rBV	1023900	1058079	24.29%	2.238%
37	12.948	1800	1804	1805	rBV	241139	226332	5.20%	0.479%
38	12.972	1805	1808	1811	rVB	781887	696309	15.99%	1.473%
39	13.113	1822	1832	1835	rBV	3787874	4156531	95.44%	8.794%
40	13.172	1839	1842	1843	rBV3	54387	47257	1.09%	0.100%
41	13.189	1843	1845	1848	rVB2	60073	65584	1.51%	0.139%
42	13.295	1860	1863	1865	rVB	158957	109512	2.51%	0.232%
43	13.319	1865	1867	1870	rVB3	94327	85783	1.97%	0.181%
44	13.360	1870	1874	1877	rBV	148797	185507	4.26%	0.392%
45	13.395	1877	1880	1884	rBV5	62655	90637	2.08%	0.192%
46	13.660	1923	1925	1928	rBV2	92040	85953	1.97%	0.182%
47	13.783	1943	1946	1948	rBV3	68537	65483	1.50%	0.139%
48	13.919	1966	1969	1972	rBV3	53534	53481	1.23%	0.113%
49	13.983	1976	1980	1984	rBV6	344151	400680	9.20%	0.848%
50	14.171	2007	2012	2014	rBV2	1375475	1518429	34.86%	3.212%
51	14.195	2014	2016	2022	rVB	434464	344769	7.92%	0.729%
52	14.260	2024	2027	2028	rBV3	63567	61773	1.42%	0.131%
53	14.277	2028	2030	2033	rVB2	68990	58272	1.34%	0.123%
54	14.307	2033	2035	2039	rBV	130406	108880	2.50%	0.230%
55	14.395	2046	2050	2054	rBV6	61751	103944	2.39%	0.220%
56	14.554	2072	2077	2079	rVB5	66508	99848	2.29%	0.211%
57	14.618	2085	2088	2092	rBV4	160686	176103	4.04%	0.373%
58	14.707	2102	2103	2106	rVB3	79407	54321	1.25%	0.115%
59	14.936	2139	2142	2147	rVB3	110200	130349	2.99%	0.276%
60	15.248	2191	2195	2198	rBV2	174892	280878	6.45%	0.594%
61	15.571	2247	2250	2257	rVB3	110454	167553	3.85%	0.354%
62	15.636	2258	2261	2265	rVB	162228	195251	4.48%	0.413%
63	15.707	2269	2273	2278	rBV2	584700	736351	16.91%	1.558%
64	16.171	2348	2352	2357	rVB8	61369	98544	2.26%	0.208%

Sum of corrected areas: 47267330

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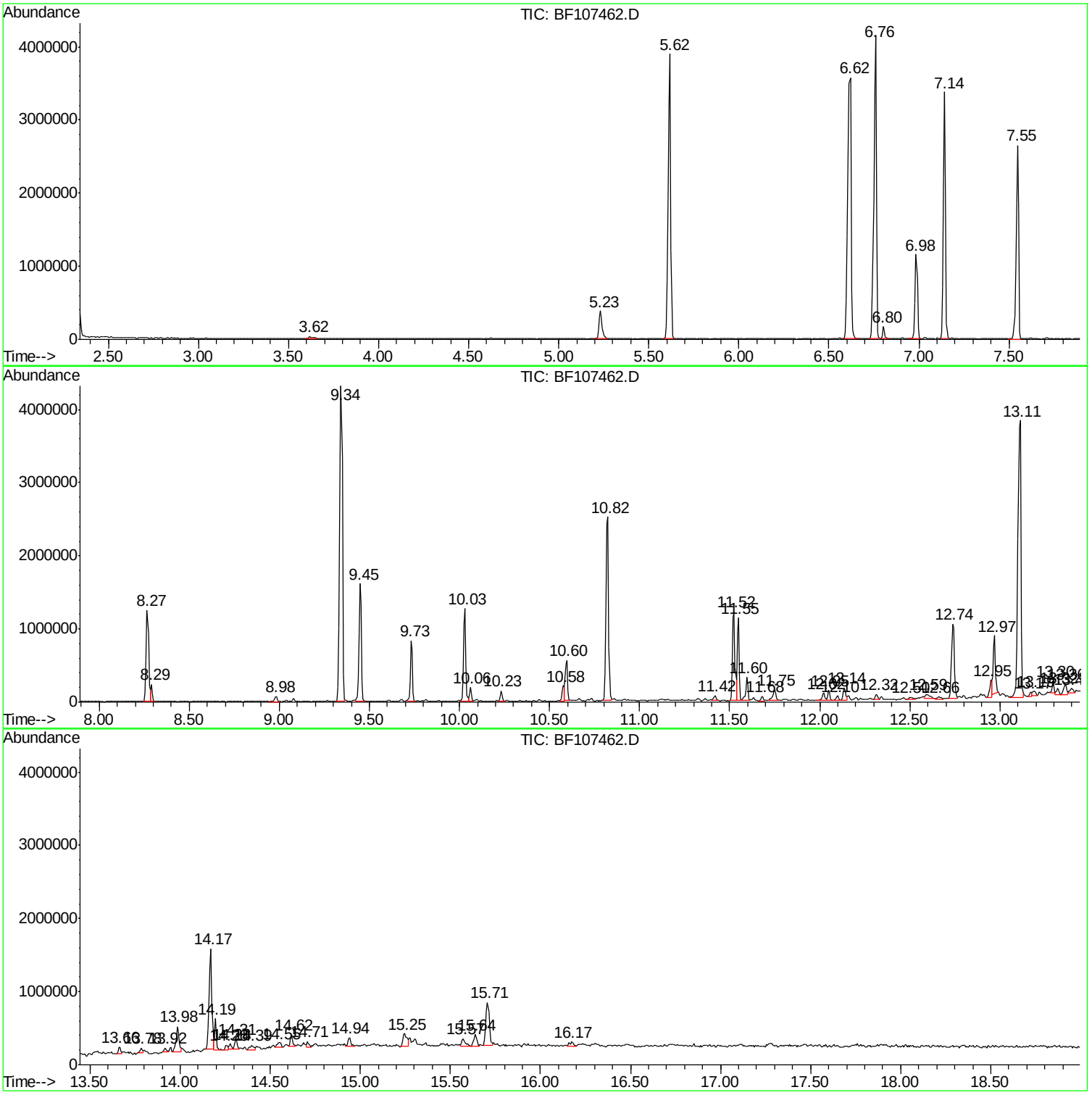
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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\BF071718\
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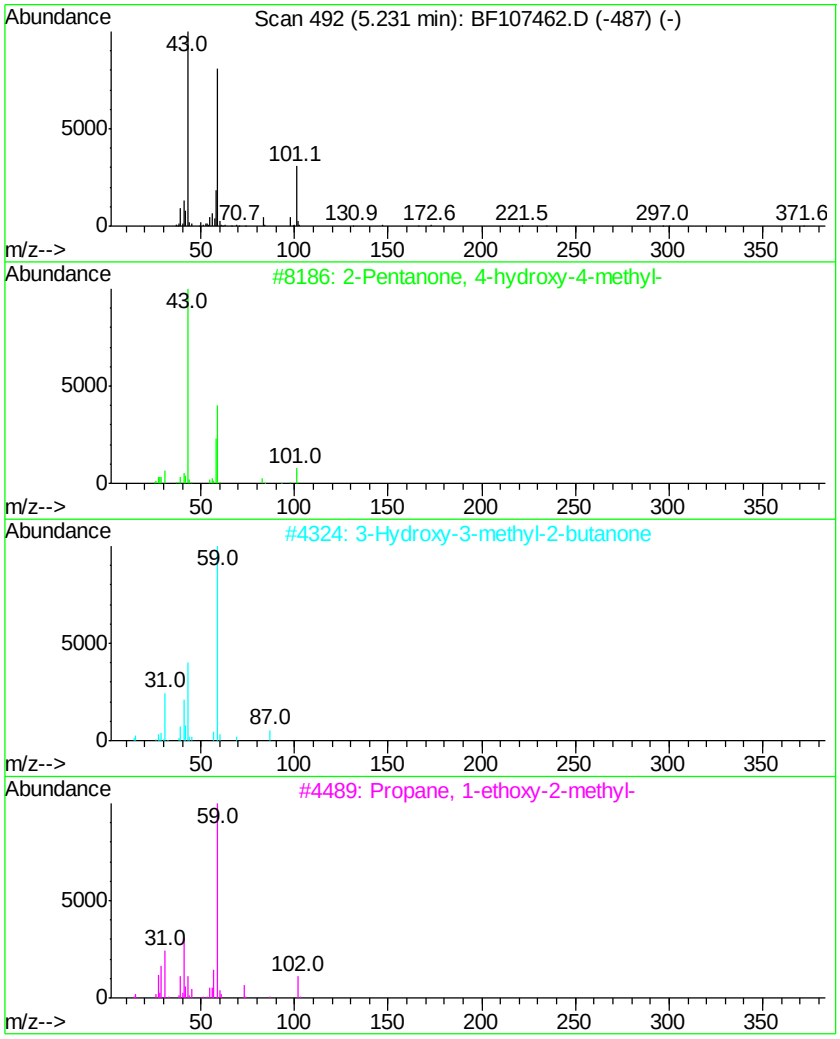
TIC Integration Parameters: LSCINT.P

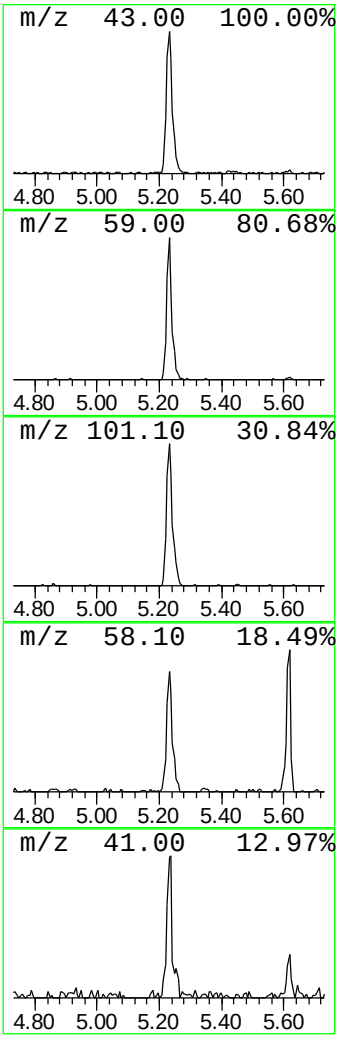
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	10.29 ng	502951	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	47
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	46
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	45
5	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	39





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\
Data File : BF107462.D
Acq On : 17 Jul 2018 21:01
Operator : JU/SJ
Sample : J3906-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

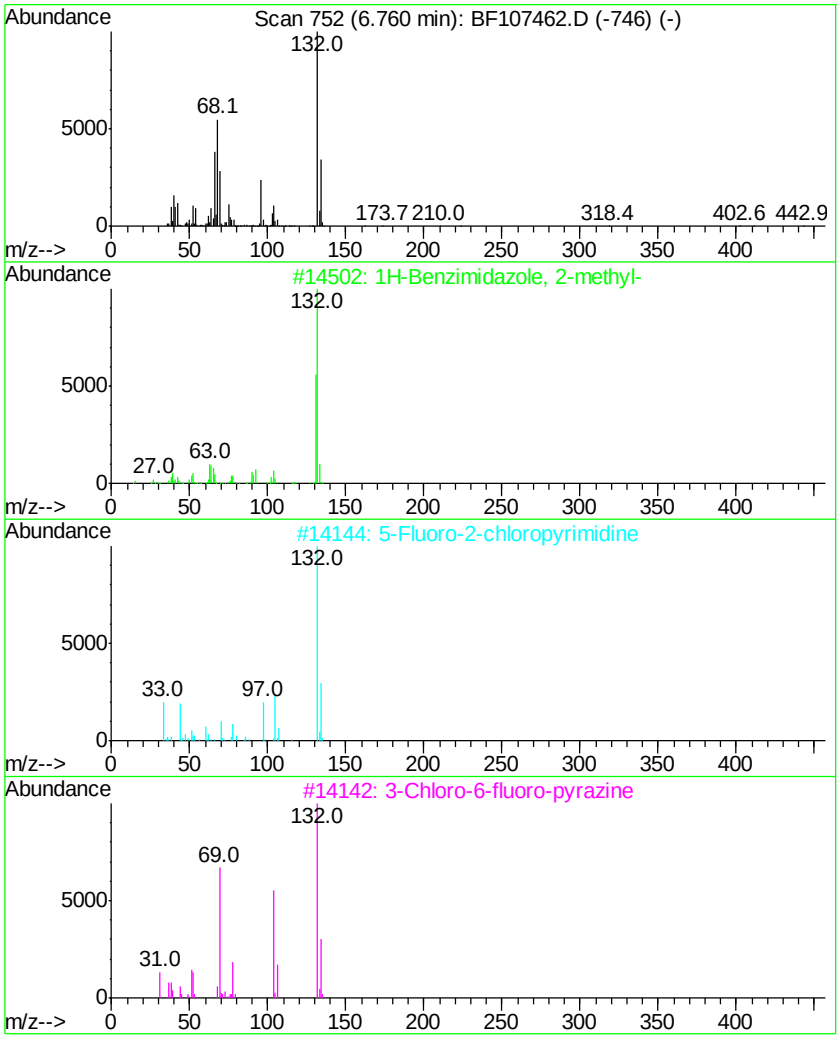
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

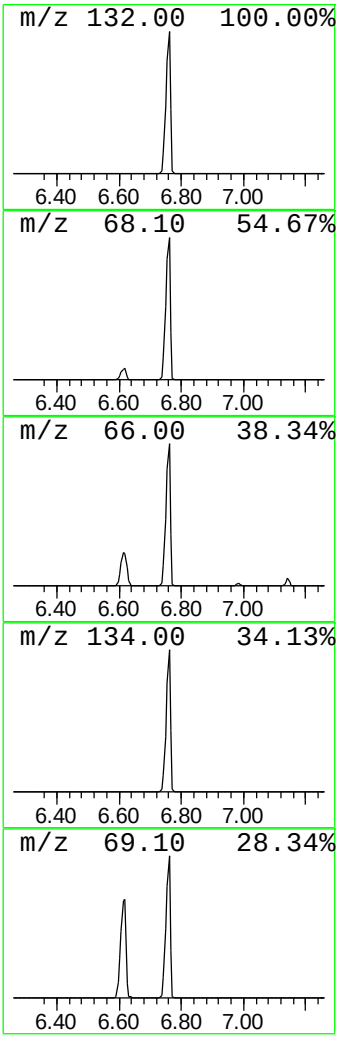
****

Peak Number 2 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	85.30 ng	4170290	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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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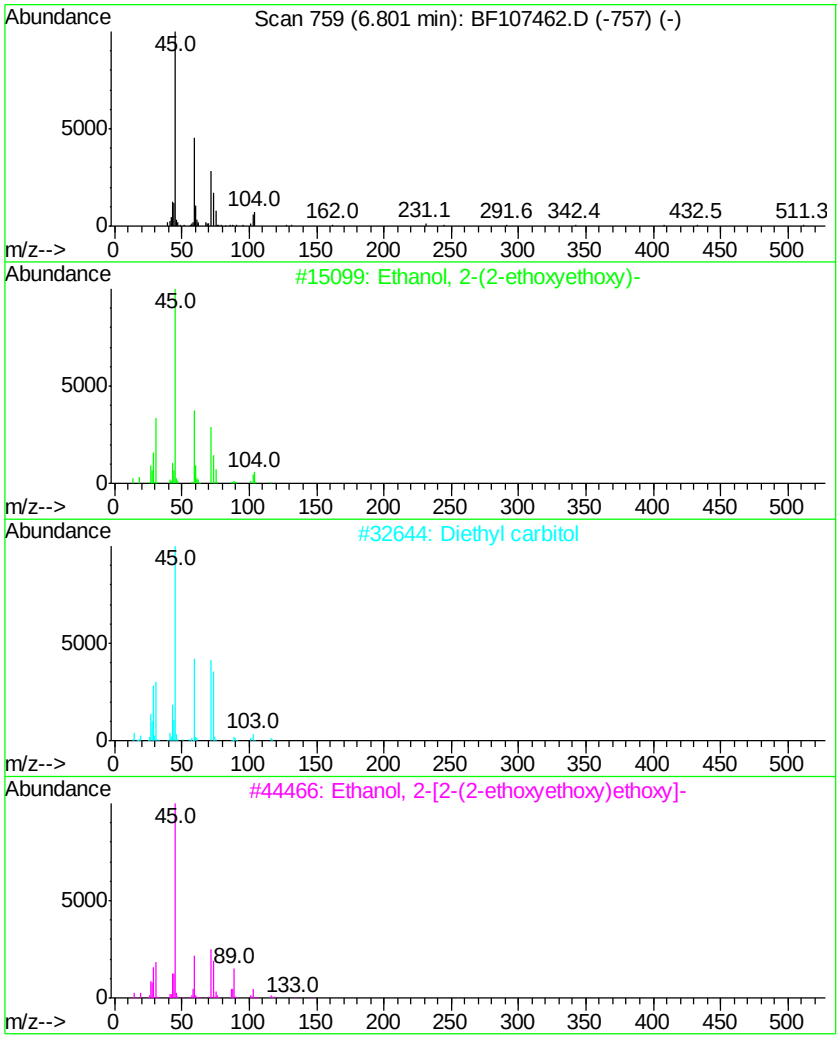
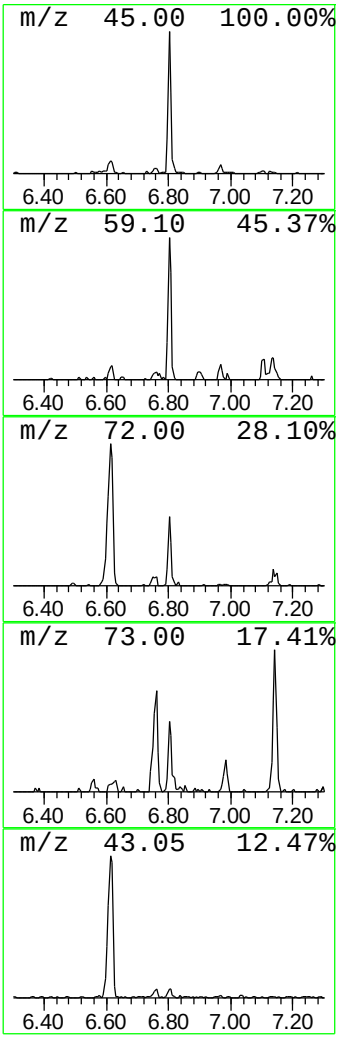
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	2.71 ng	132536	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	59
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	53
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
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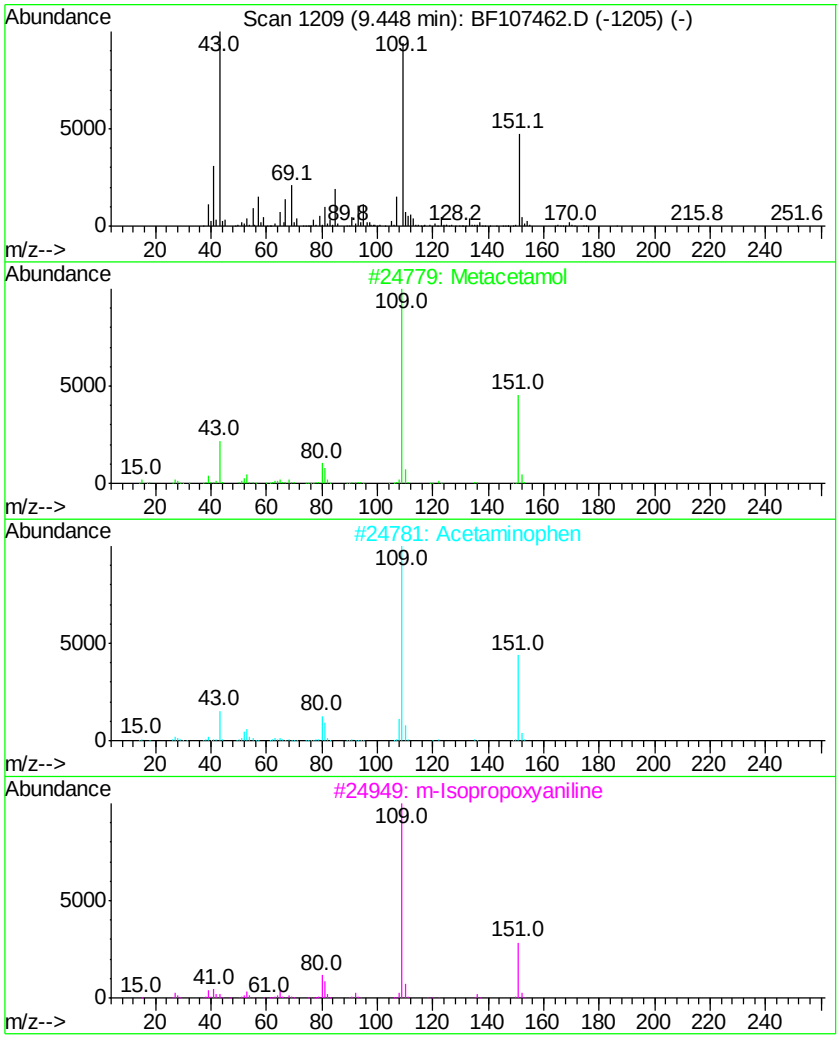
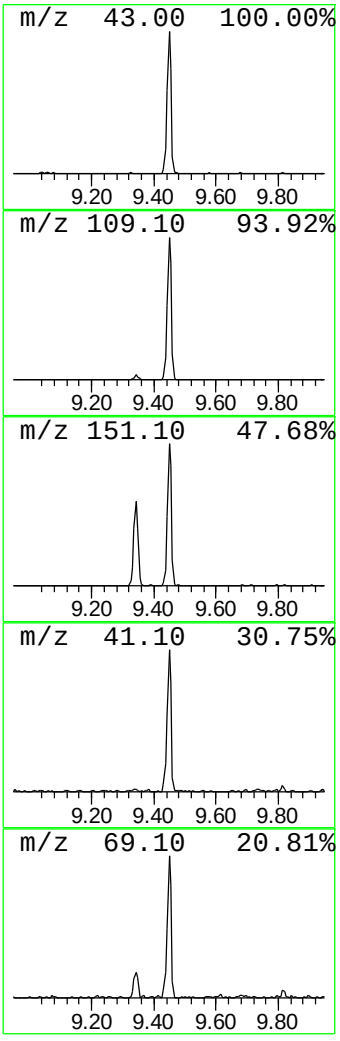
Peak Number 5 Metacetamol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.45	27.67 ng	1598250	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	58
2	Acetaminophen	151	C8H9NO2	000103-90-2	53
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
4	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53
5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	50





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

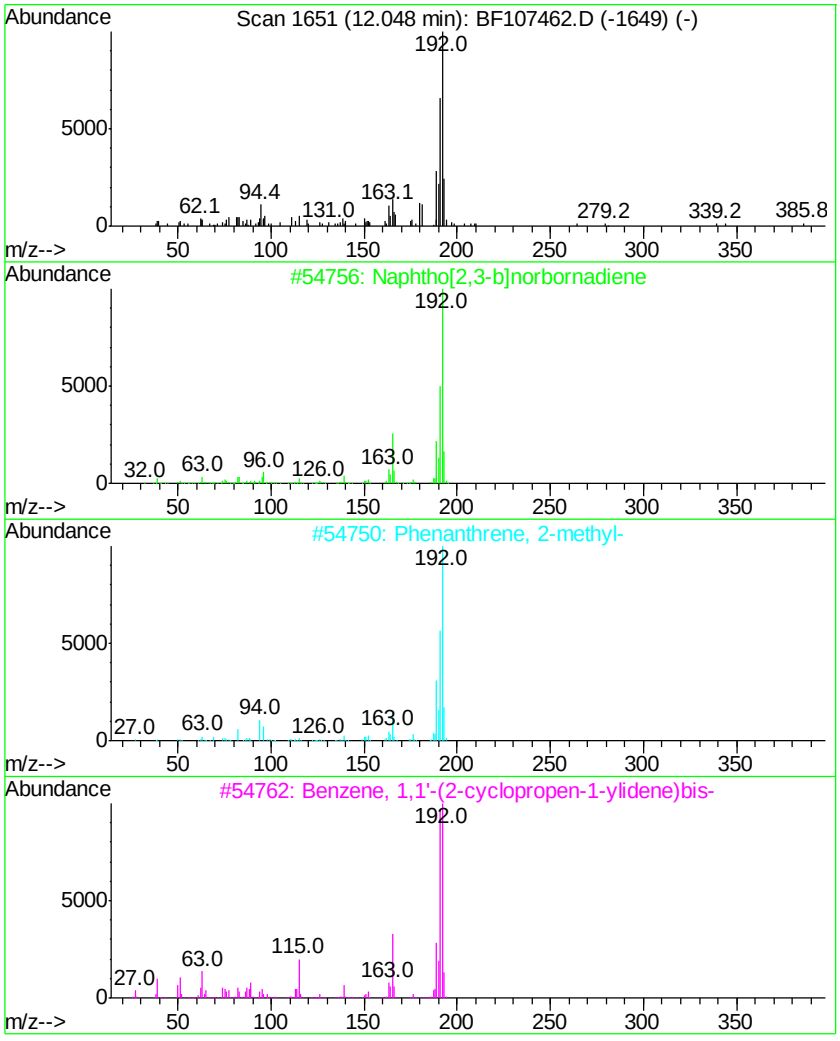
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

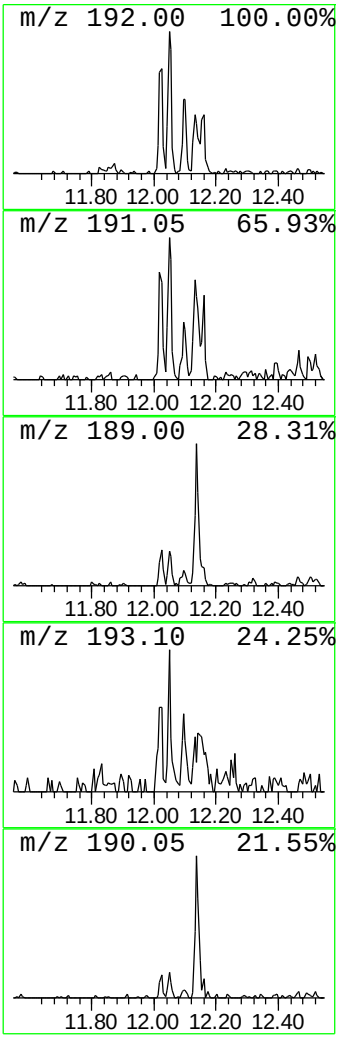
****

Peak Number 7 Naphtho[2,3-b]norbornadiene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.00 ng	123229	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	70
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	62
3	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	60
4	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	60
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	58





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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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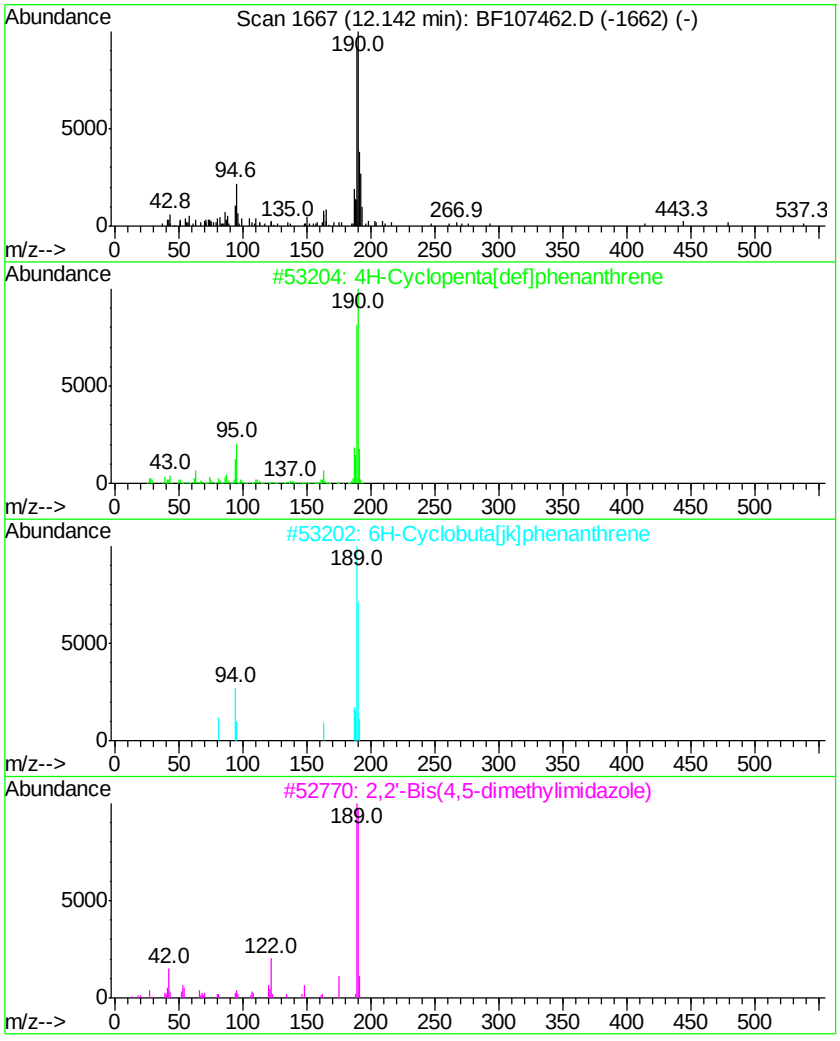
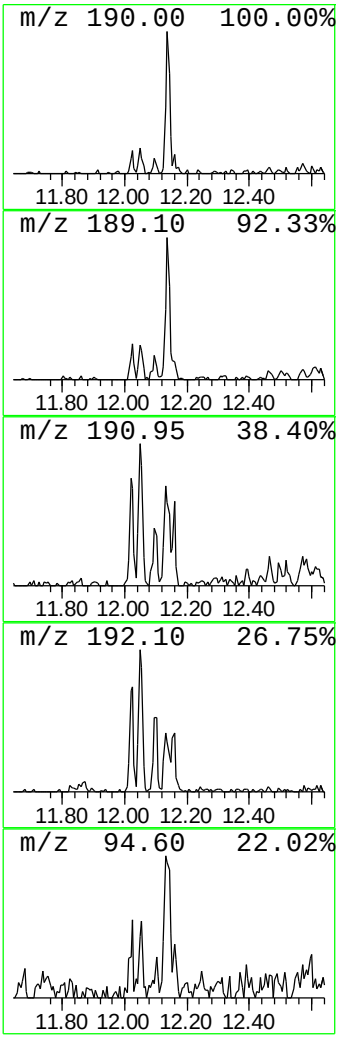
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	3.35 ng	206096	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	6-Bromo-9-phenanthrene diazometh...	324	C16H9BrN2O	1000254-49-2	25
5	1-Aminocyclopentanecarboxylic ac...	319	C15H26ClNO4	1000329-16-6	16





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Sample : J3906-01
Misc :
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Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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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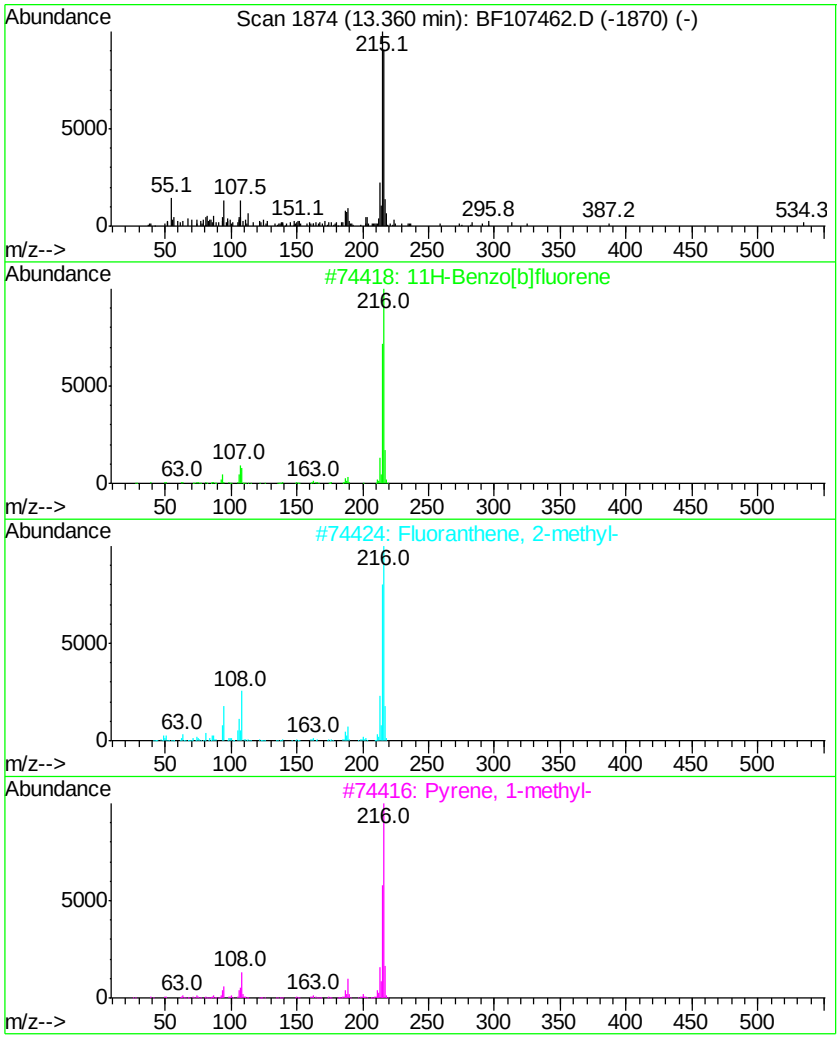
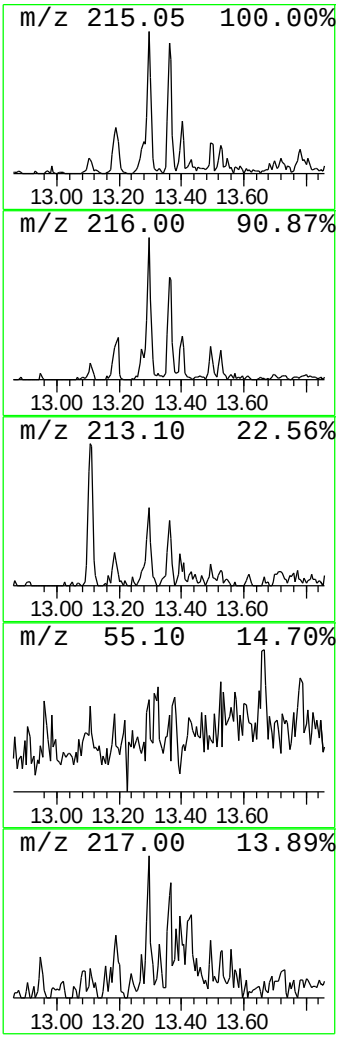
Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	2.44 ng	185507	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	72
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	59
4	2-Chloro-7-phenyltropone	216	C13H9ClO	090128-01-1	53
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	53





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Data File : BF107462.D
Acq On : 17 Jul 2018 21:01
Operator : JU/SJ
Sample : J3906-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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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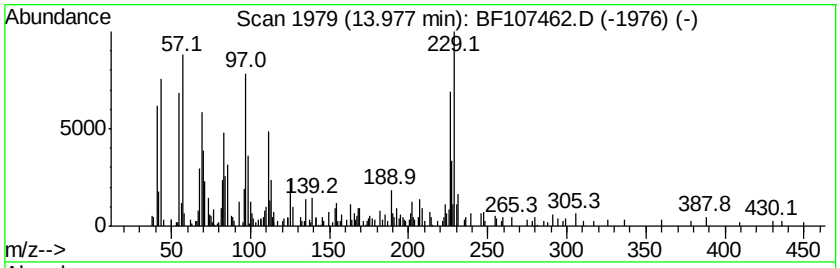
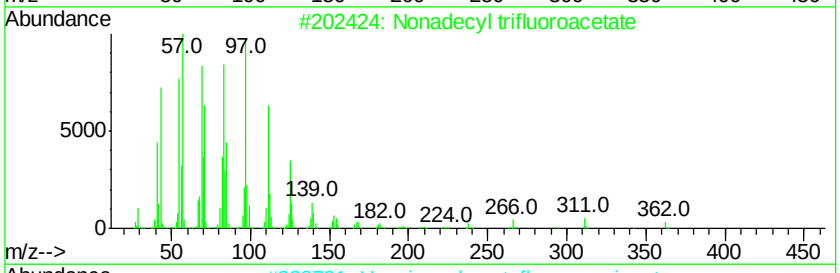
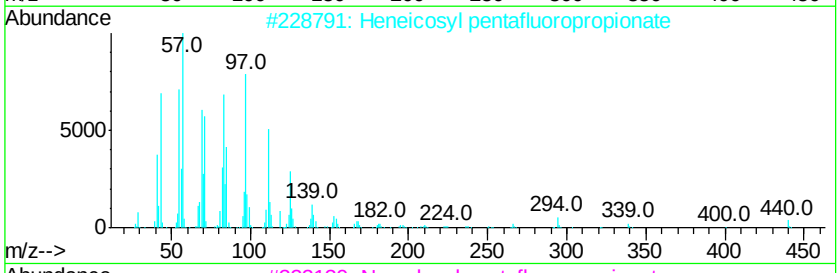
Peak Number 10 Nonadecyl trifluoroacetate Concentration Rank 5

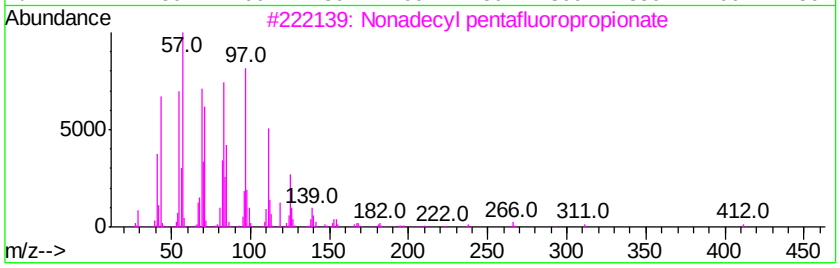
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	5.28 ng	400680	Chrysene-d12	14.17

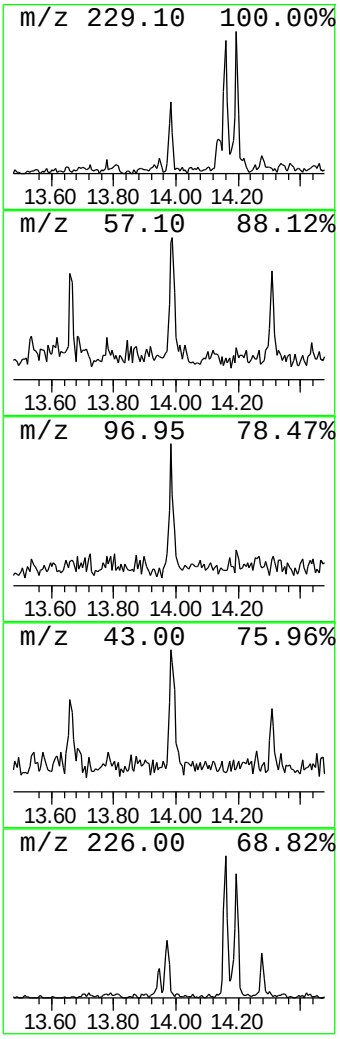
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	93
2	Heneicosyl pentafluoropropionate	458	C24H43F5O2	1000351-81-1	93
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	86
4	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	86
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	86











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Data File : BF107462.D
Acq On : 17 Jul 2018 21:01
Operator : JU/SJ
Sample : J3906-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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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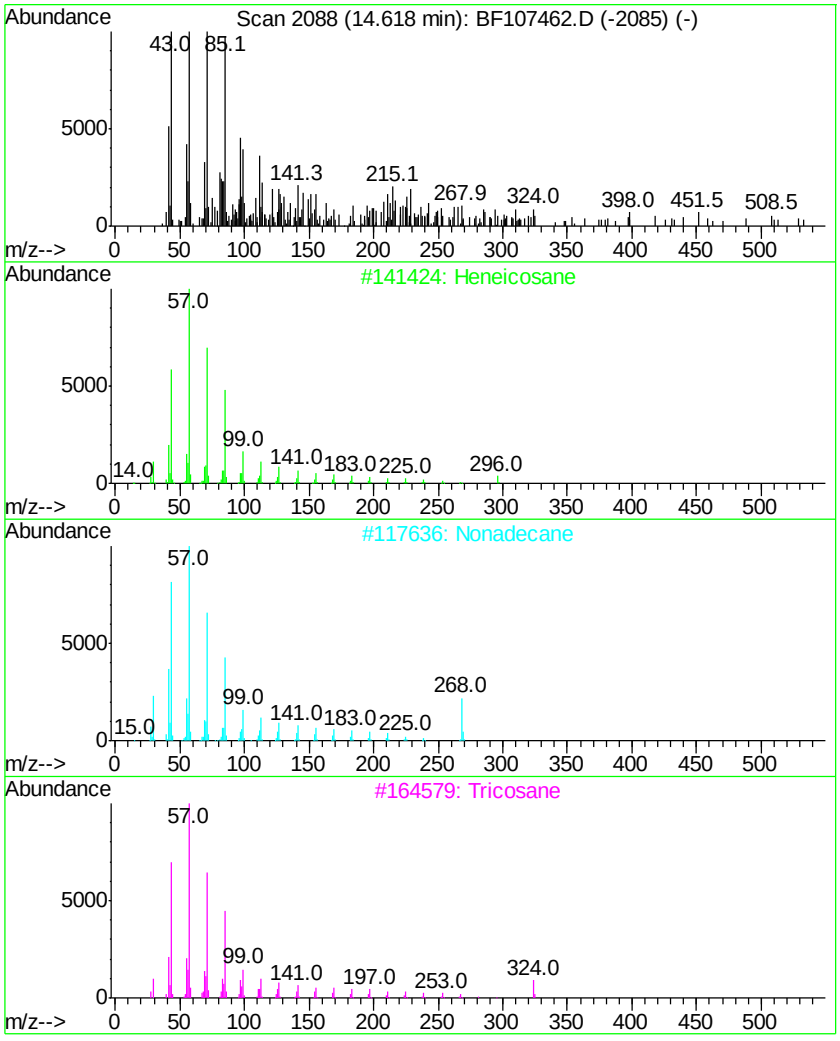
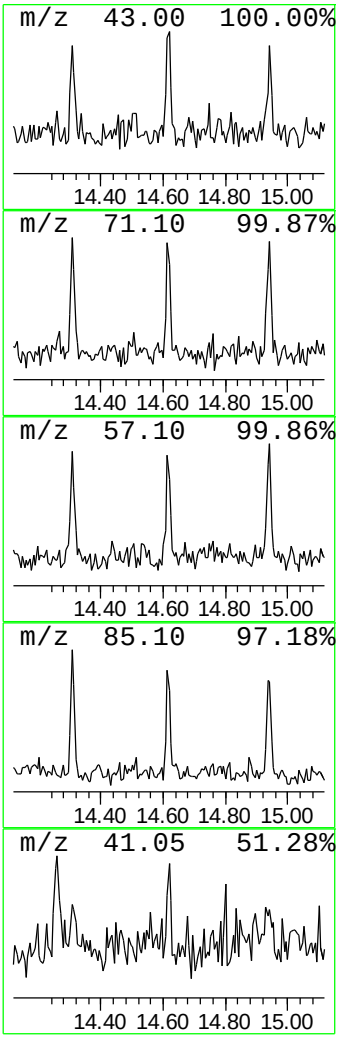
Peak Number 11 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.32 ng	176103	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Nonadecane	268	C19H40	000629-92-5	76
3	Tricosane	324	C23H48	000638-67-5	74
4	Heptadecane	240	C17H36	000629-78-7	74
5	1-Iodoundecane	282	C11H23I	004282-44-4	68





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Data File : BF107462.D
Acq On : 17 Jul 2018 21:01
Operator : JU/SJ
Sample : J3906-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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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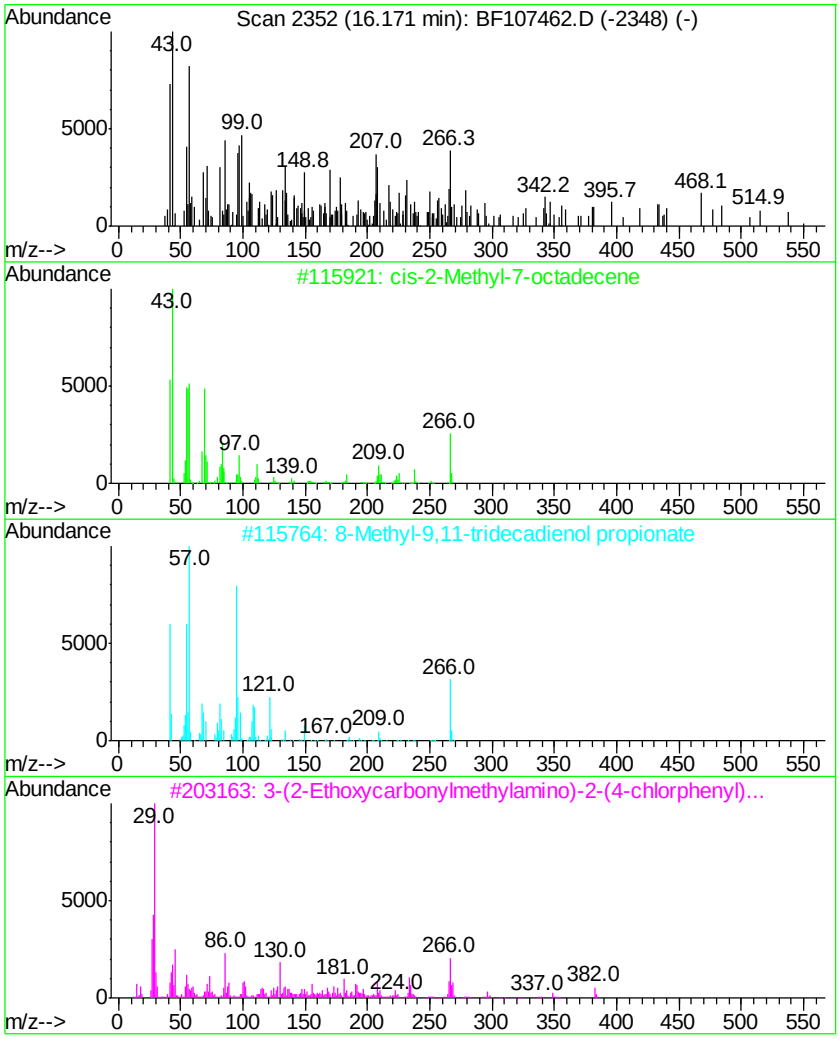
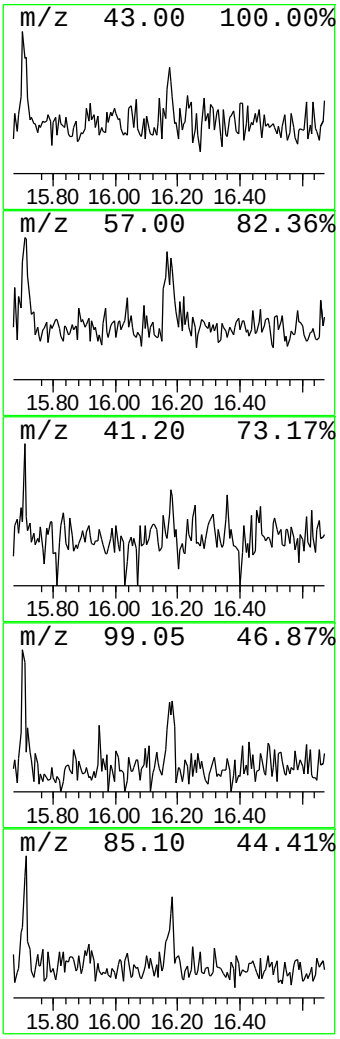
Peak Number 13 unknown16.17 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.68 ng	98544	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-2-Methyl-7-octadecene	266	C19H38	035354-39-3	25
2	8-Methyl-9,11-tridecadienol prop...	266	C17H30O2	1000130-96-9	25
3	3-(2-Ethoxycarbonylmethylamino)-...	382	C18H23ClN2O3S	1000287-30-0	22
4	Acetonitrile, 2-[3-(2,6-dichloro...	266	C12H8Cl2N2O	1000264-41-5	22
5	Dihydroartemisinin, 5-deshydroxy...	266	C15H22O4	082596-30-3	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071718\
Data File : BF107462.D
Acq On : 17 Jul 2018 21:01
Operator : JU/SJ
Sample : J3906-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CB-7-8-6-ST-WW-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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...	5.23	10.3	ng	502951	1	6.98	977753	20.0
unknown6.76	6.76	85.3	ng	4170290	1	6.98	977753	20.0
Ethanol, 2-(2-eth...	6.80	2.7	ng	132536	1	6.98	977753	20.0
Metacetamol	9.45	27.7	ng	1598250	3	10.03	1155090	20.0
Naphtho[2,3-b]nor...	12.05	2.0	ng	123229	4	11.52	1229400	20.0
4H-Cyclopenta[def...	12.14	3.4	ng	206096	4	11.52	1229400	20.0
11H-Benzo[b]fluorene	13.36	2.4	ng	185507	5	14.17	1518430	20.0
Nonadecyl trifluo...	13.98	5.3	ng	400680	5	14.17	1518430	20.0
Heneicosane	14.62	2.3	ng	176103	5	14.17	1518430	20.0
unknown16.17	16.17	2.7	ng	98544	6	15.71	736351	20.0