LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103380.D
Acq On : 2 Mar 2018 21:55
Operator : SJ/JU
Sample : J1721-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

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:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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	2.134	3	8	17	rVB	212182	289883	8.91%	0.912%
2	5.110	511	514	526	rVB	86707	118120	3.63%	0.371%
3	5.504	577	581	602	rVB	3010018	3253211	100.00%	10.230%
4	6.516	748	753	771	rBV	2802118	3232921	99.38%	10.167%
5	6.651	771	776	779	rVV	3198496	3073615	94.48%	9.666%
6	6.698	781	784	790	rVB2	38508	40510	1.25%	0.127%
7	6.875	811	814	820	rBV	1184566	959632	29.50%	3.018%
8	7.034	837	841	844	rBV	2585229	2347401	72.16%	7.382%
9	7.439	906	910	926	rBV	1927305	2118990	65.14%	6.664%
10	8.157	1029	1032	1052	rVB	1212775	1335305	41.05%	4.199%
11	8.875	1151	1154	1161	rBV	38737	47638	1.46%	0.150%
12	9.233	1211	1215	1224	rBV	2938359	2765011	84.99%	8.695%
13	9.304	1224	1227	1230	rVB	74331	72802	2.24%	0.229%
14	9.628	1276	1282	1288	rBV	195945	245395	7.54%	0.772%
15	9.781	1304	1308	1312	rBV	53207	65345	2.01%	0.205%
16	9.833	1313	1317	1320	rVB	117093	104410	3.21%	0.328%
17	9.916	1325	1331	1335	rVV	1186191	1113653	34.23%	3.502%
18	9.951	1335	1337	1344	rVB	71300	80634	2.48%	0.254%
19	10.069	1352	1357	1359	rBV4	24228	33281	1.02%	0.105%
20	10.122	1363	1366	1369	rVV2	47758	56713	1.74%	0.178%
21	10.151	1369	1371	1375	rVB3	37684	45276	1.39%	0.142%
22	10.233	1381	1385	1388	rBV2	24433	35021	1.08%	0.110%
23	10.328	1395	1401	1405	rBV	145864	167471	5.15%	0.527%
24	10.469	1422	1425	1431	rVB3	43969	45726	1.41%	0.144%
25	10.551	1434	1439	1441	rBV2	53746	61557	1.89%	0.194%
26	10.710	1462	1466	1479	rBV	1249516	1370423	42.13%	4.310%
27	10.804	1479	1482	1492	rVB	131191	194710	5.99%	0.612%
28	11.251	1556	1558	1561	rBV2	78912	77508	2.38%	0.244%
29	11.410	1581	1585	1587	rBV	968666	854602	26.27%	2.687%
30	11.433	1587	1589	1594	rVV	501319	435349	13.38%	1.369%
31	11.486	1595	1598	1603	rVV	129354	128929	3.96%	0.405%
32	11.680	1629	1631	1633	rVB	48762	35355	1.09%	0.111%
33	11.922	1668	1672	1674	rBV2	109050	146066	4.49%	0.459%
34	11.939	1674	1675	1680	rVB2	97636	86261	2.65%	0.271%

LSC Area Percent Report

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Operator : SJ/JU
Sample : J1721-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

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 >
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.992	1681	1684	1687	rVB	33578	34339	1.06%	0.108%
36	12.027	1687	1690	1692	rBV	118679	121985	3.75%	0.384%
37	12.086	1698	1700	1704	rBV3	42570	43001	1.32%	0.135%
38	12.204	1718	1720	1724	rBV	50825	50941	1.57%	0.160%
39	12.245	1724	1727	1731	rVB3	46781	50136	1.54%	0.158%
40	12.463	1761	1764	1768	rBV2	70325	103816	3.19%	0.326%
41	12.557	1777	1780	1782	rBV2	50157	58431	1.80%	0.184%
42	12.627	1789	1792	1796	rBV	782026	743557	22.86%	2.338%
43	12.863	1825	1832	1837	rBV	814806	938580	28.85%	2.952%
44	12.992	1850	1854	1858	rBV	1689149	1724257	53.00%	5.422%
45	13.069	1865	1867	1873	rBV3	44978	84144	2.59%	0.265%
46	13.186	1885	1887	1889	rVB	88451	63115	1.94%	0.198%
47	13.257	1896	1899	1901	rBV	63567	56115	1.72%	0.176%
48	13.292	1903	1905	1907	rVB2	56479	46200	1.42%	0.145%
49	13.386	1919	1921	1923	rBV	46743	34059	1.05%	0.107%
50	13.704	1973	1975	1978	rVB	66437	51693	1.59%	0.163%
51	13.810	1991	1993	1996	rBV	74000	68282	2.10%	0.215%
52	13.874	2000	2004	2008	rBV3	380134	437626	13.45%	1.376%
53	14.063	2031	2036	2039	rBV2	823982	1076237	33.08%	3.384%
54	14.092	2039	2041	2044	rVB	347368	280139	8.61%	0.881%
55	15.133	2214	2218	2220	rBV	241648	334713	10.29%	1.053%
56	15.574	2290	2293	2297	rVB2	313562	359078	11.04%	1.129%

Sum of corrected areas: 31799168

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Misc :
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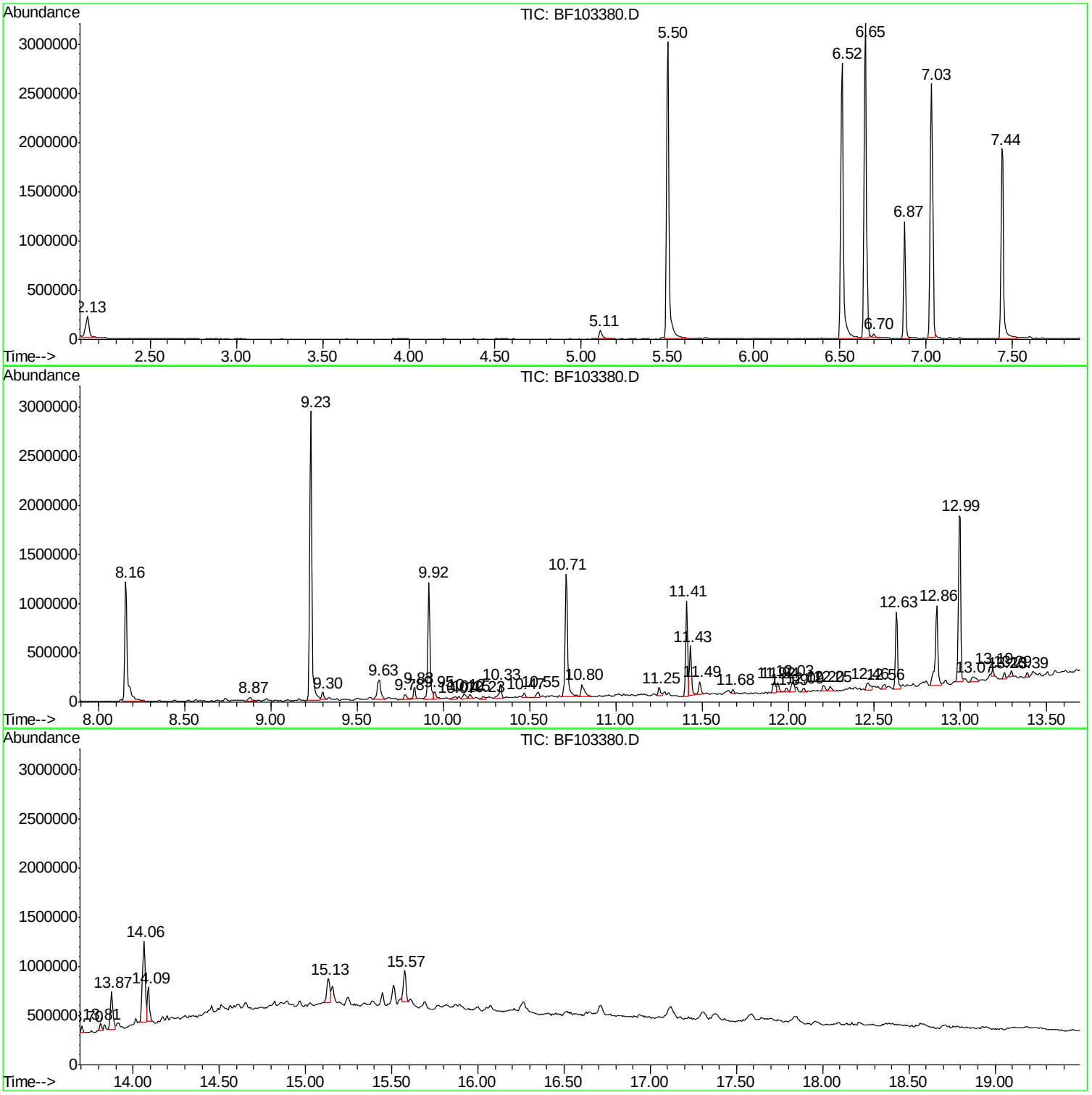
Instrument :
BNA_F
ClientSampleId :
SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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Sample : J1721-13
Misc :
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Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

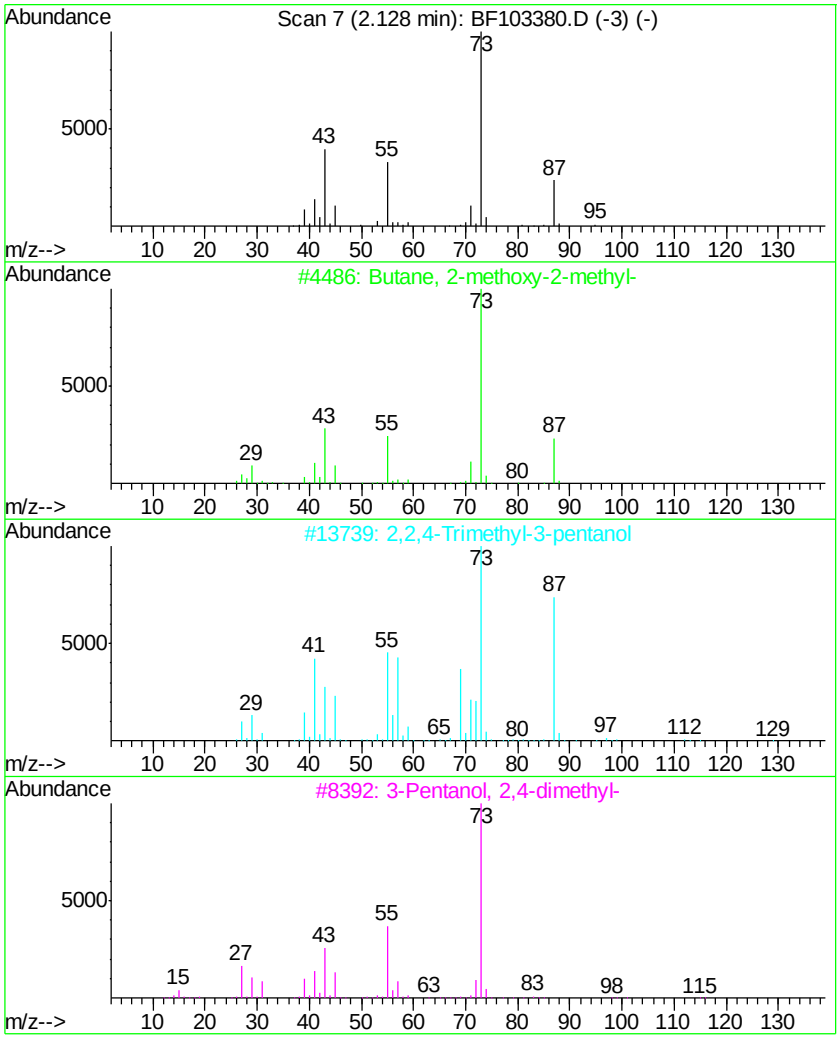
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

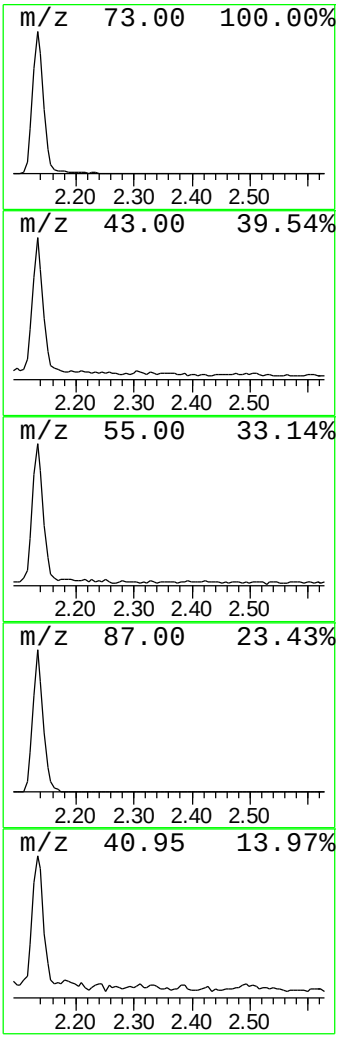
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	6.04 ng	289883	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25





Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103380.D
Acq On : 2 Mar 2018 21:55
Operator : SJ/JU
Sample : J1721-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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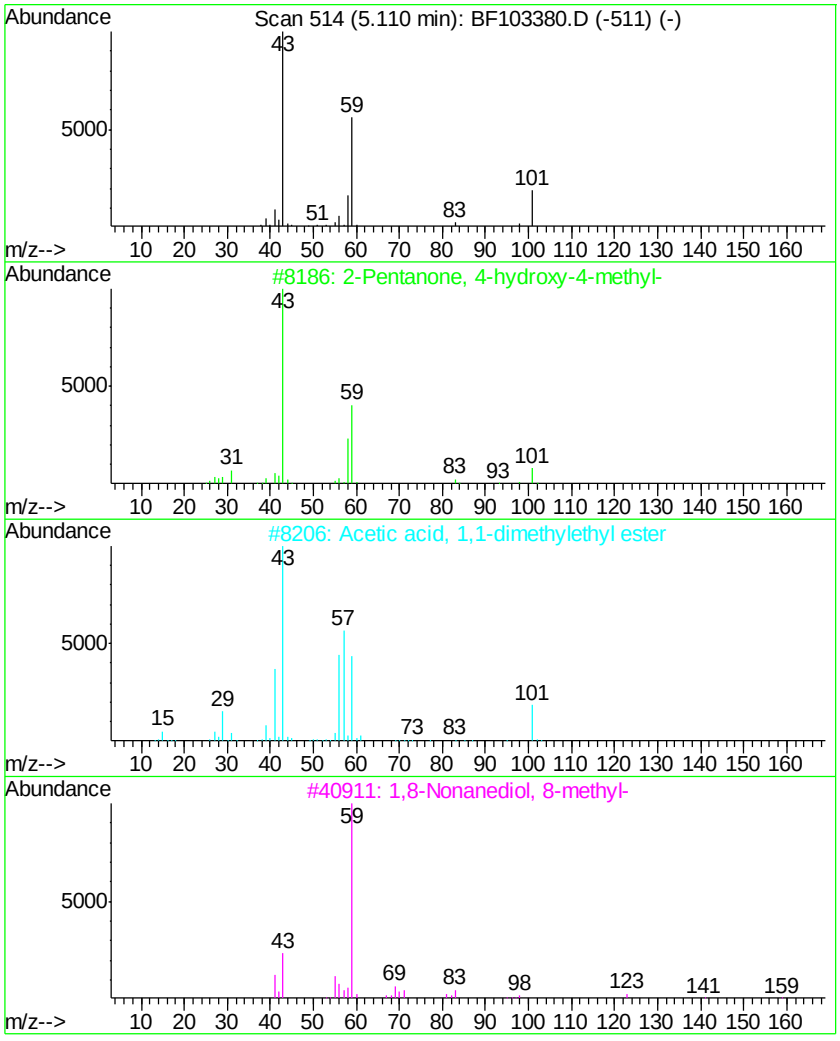
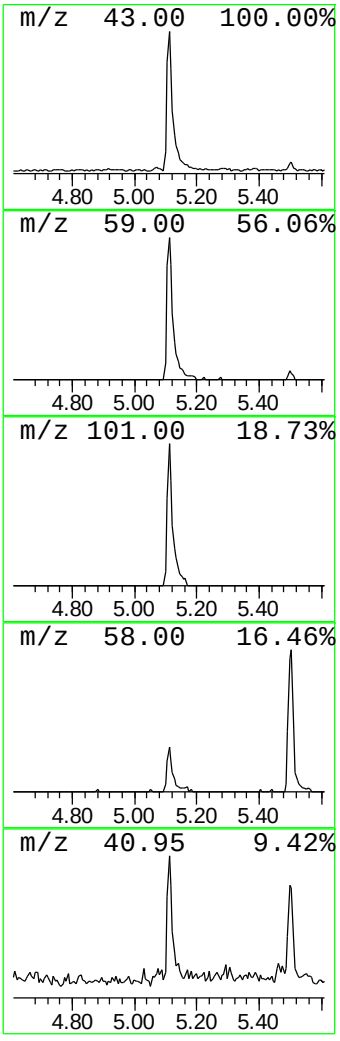
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.46 ng	118120	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103380.D
Acq On : 2 Mar 2018 21:55
Operator : SJ/JU
Sample : J1721-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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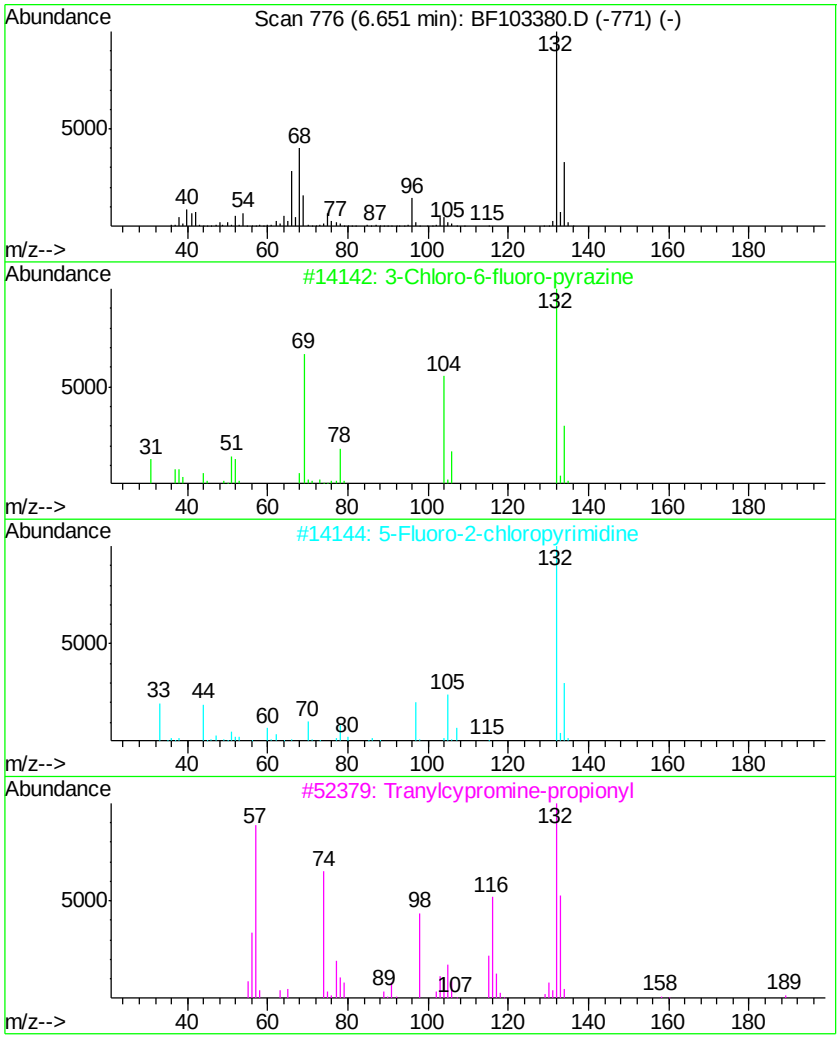
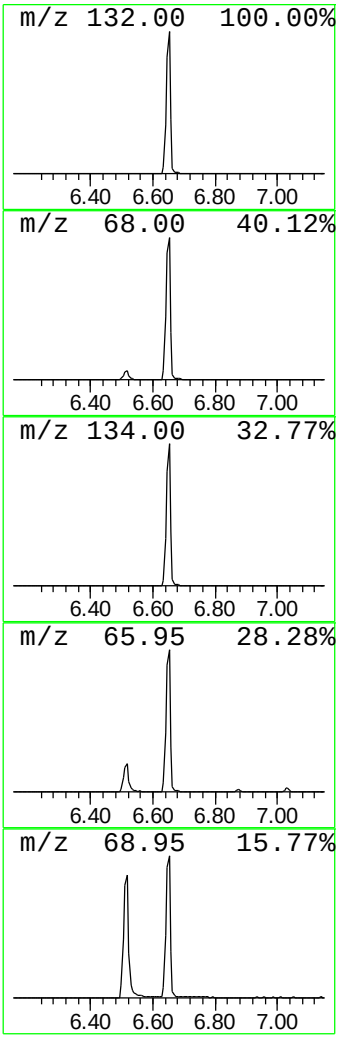
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	64.06 ng	3073620	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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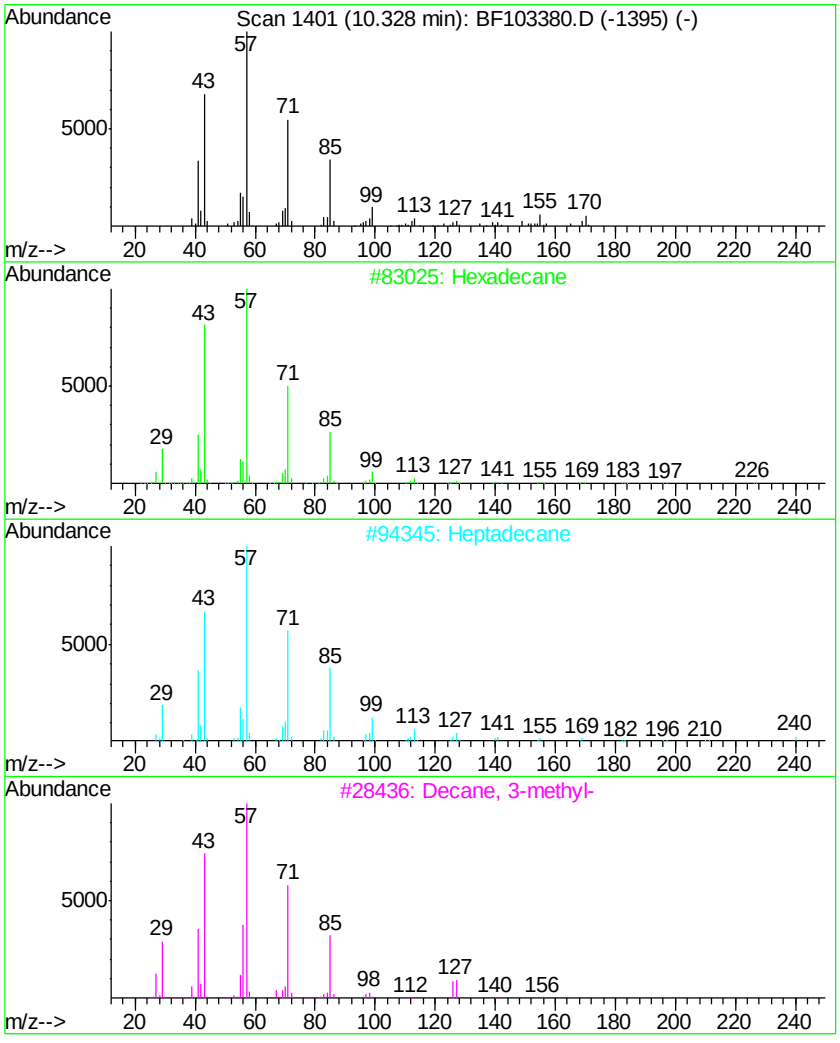
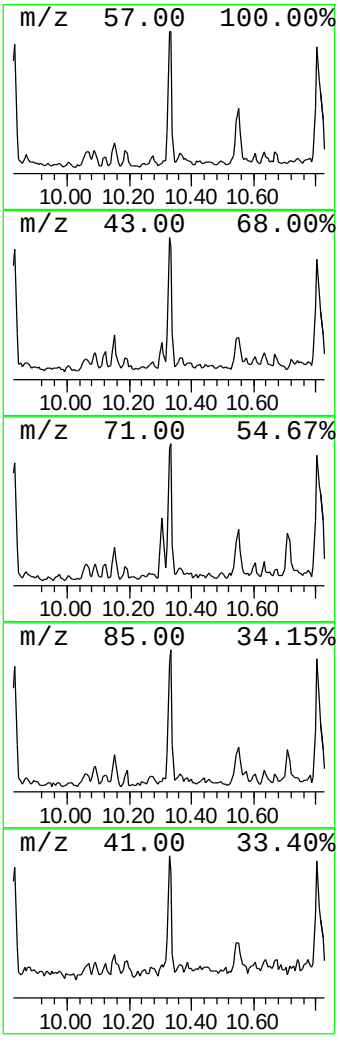
Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.01 ng	167471	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Heptadecane	240	C17H36	000629-78-7	86
3	Decane, 3-methyl-	156	C11H24	013151-34-3	81
4	Pentadecane	212	C15H32	000629-62-9	80
5	Tridecane	184	C13H28	000629-50-5	80





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
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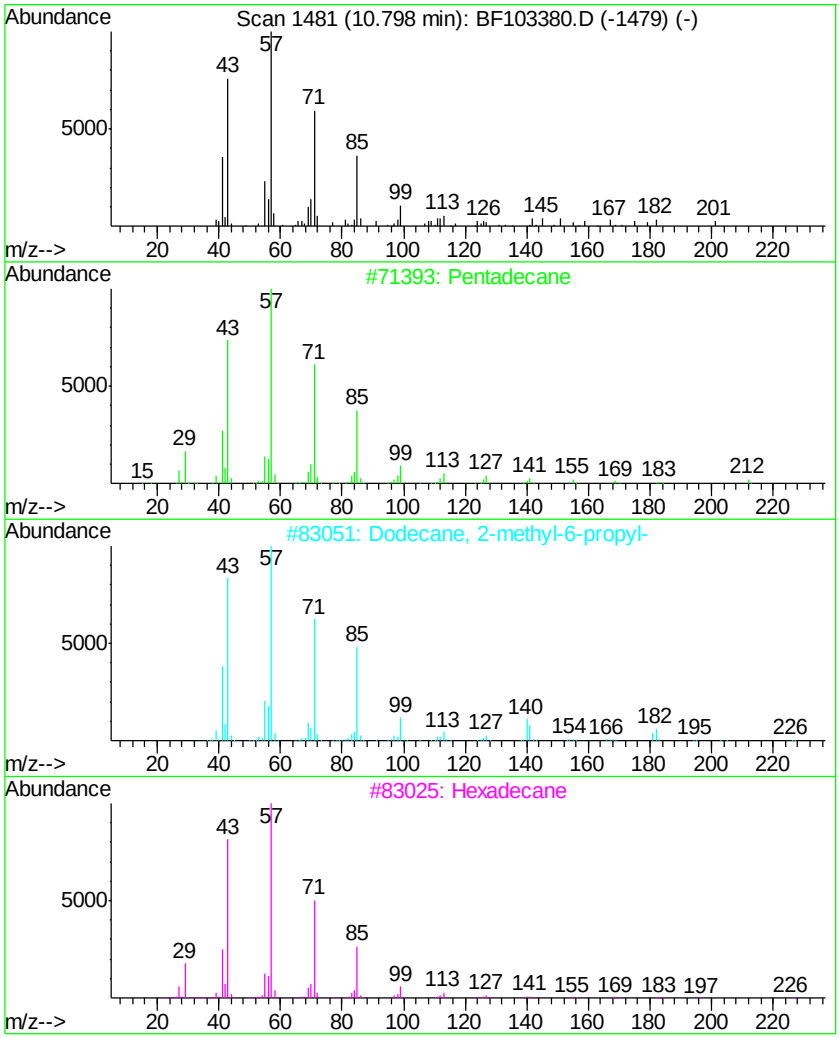
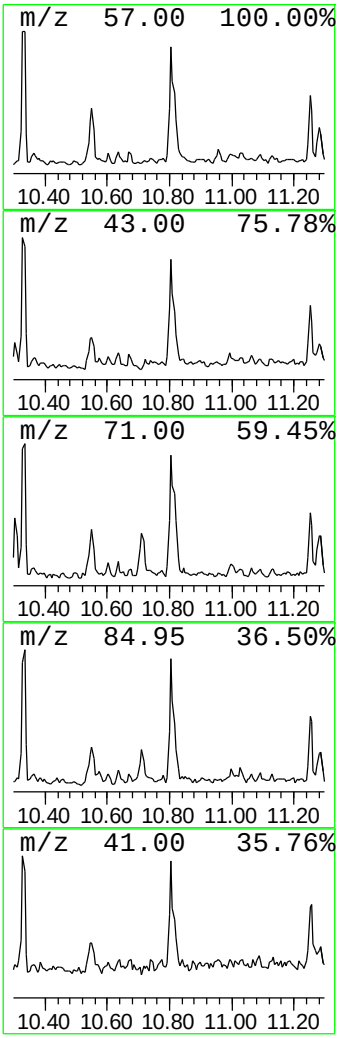
Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	4.56 ng	194710	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	83
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Hexadecane	226	C16H34	000544-76-3	72
4	Eicosane	282	C20H42	000112-95-8	72
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59





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Instrument : BNA_F
ClientSampleId : SP-46

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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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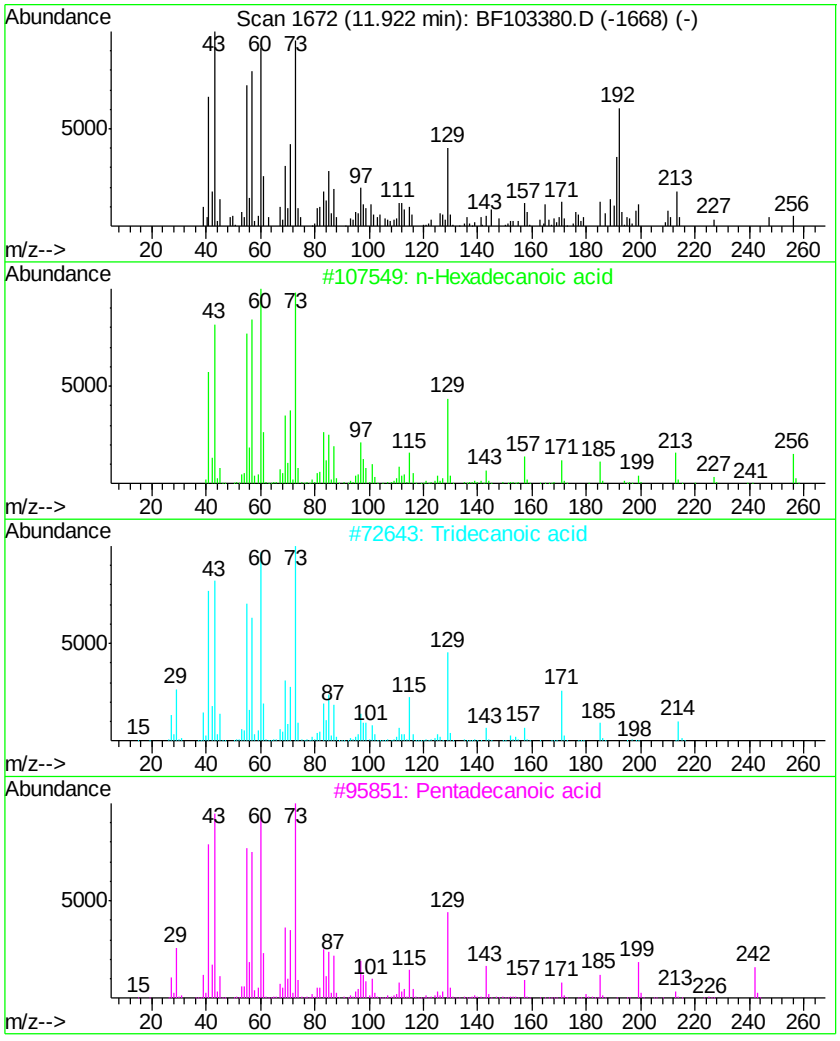
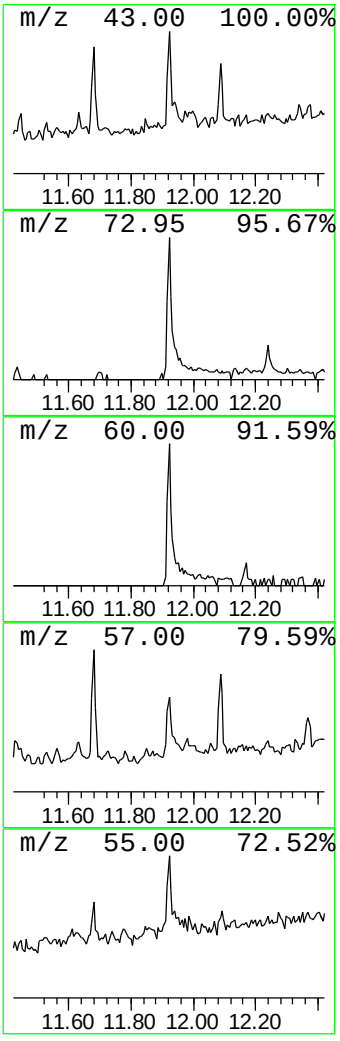
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.42 ng	146066	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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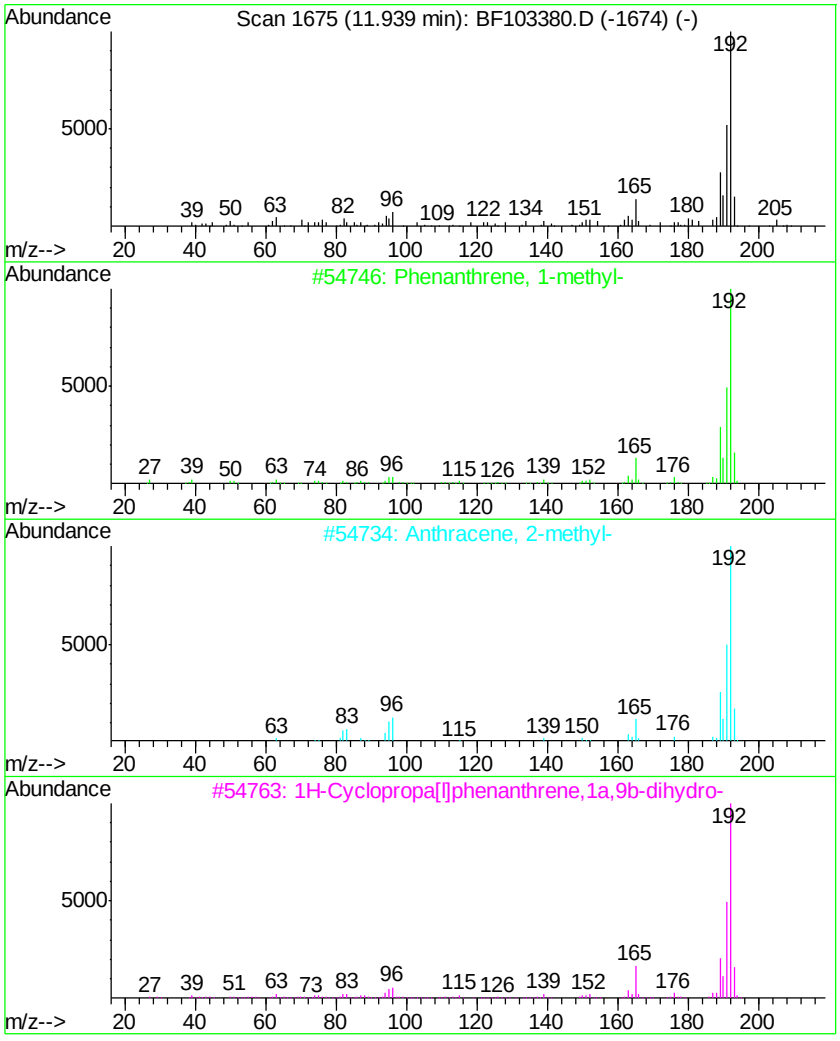
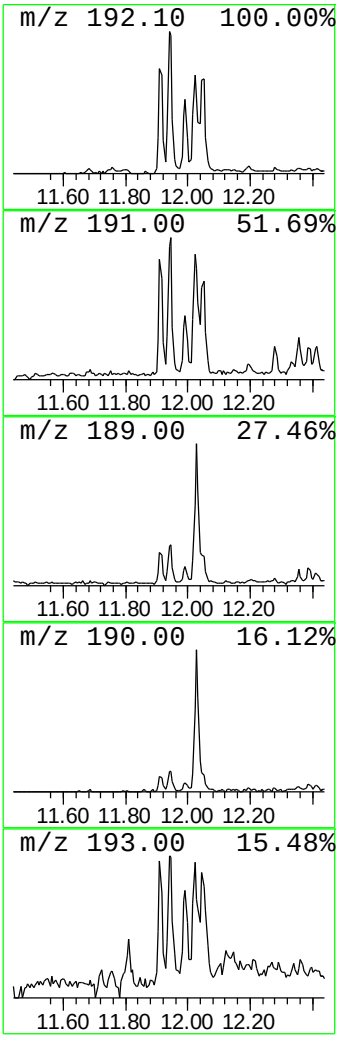
Peak Number 8 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.02 ng	86261	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91





Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103380.D
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Sample : J1721-13
Misc :
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Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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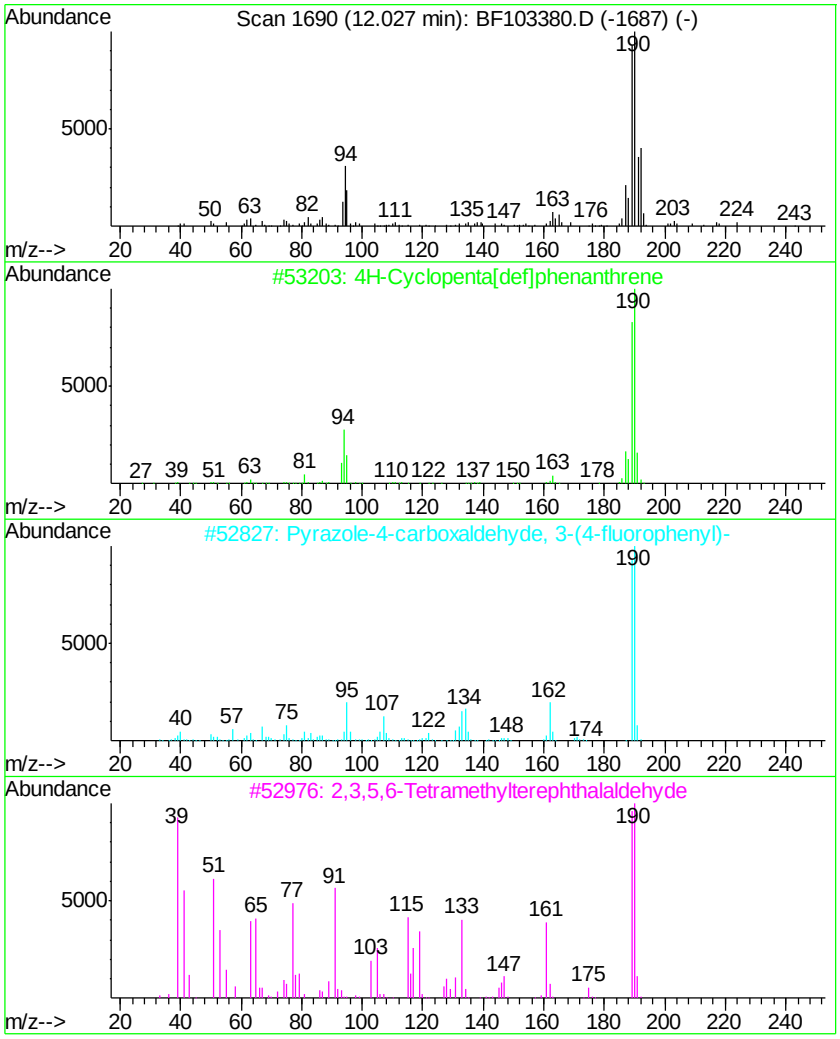
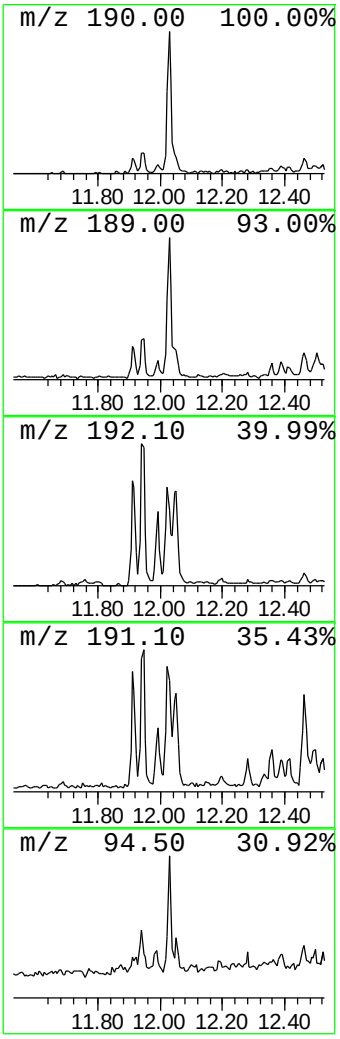
Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	2.85 ng	121985	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	95
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	47
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40





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Acq On : 2 Mar 2018 21:55
Operator : SJ/JU
Sample : J1721-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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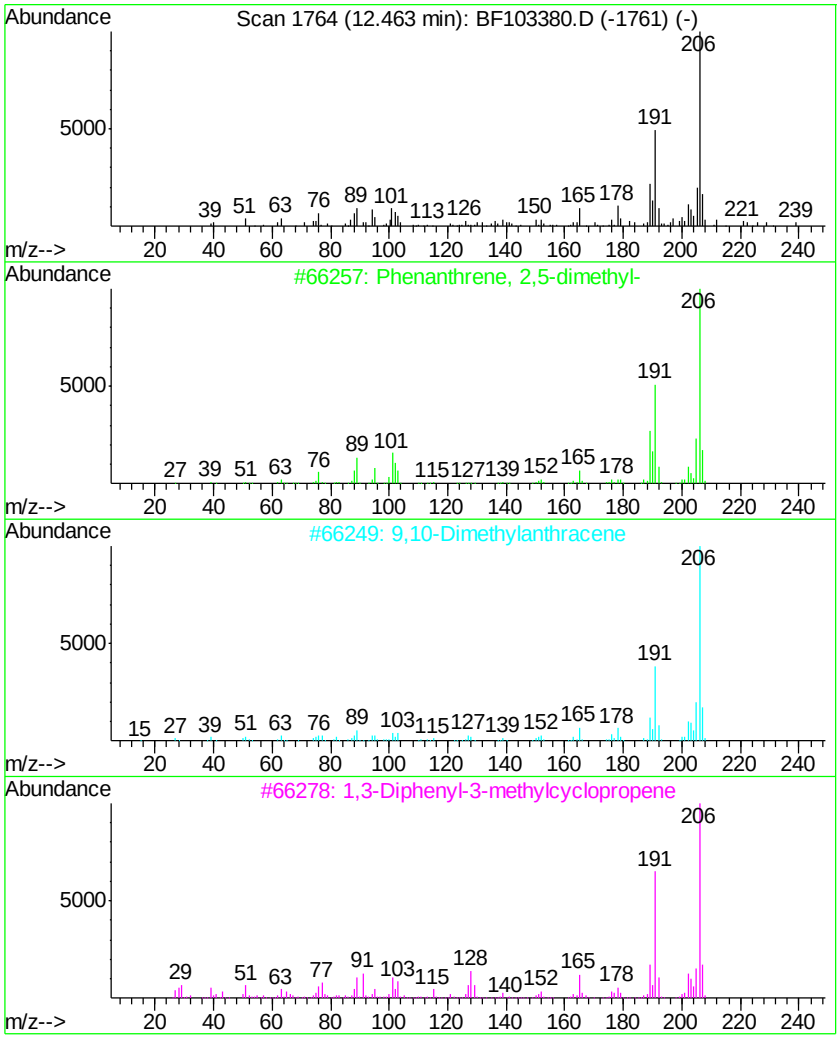
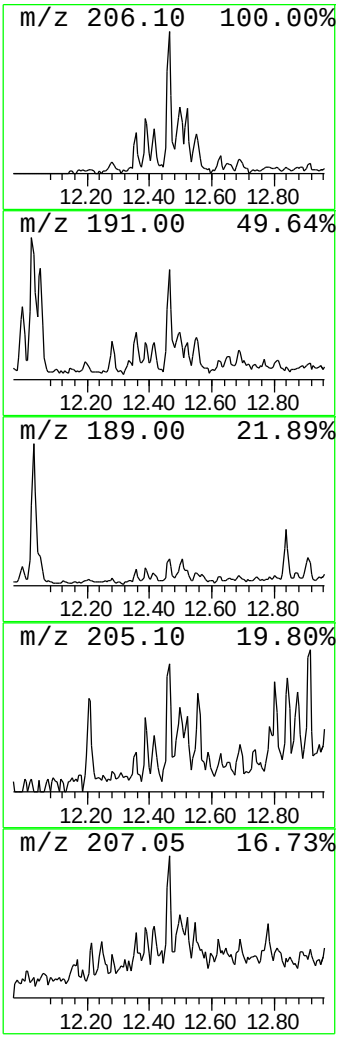
Peak Number 10 Phenanthrene, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	2.43 ng	103816	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	98
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	95
3	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	93
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	91





Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103380.D
Acq On : 2 Mar 2018 21:55
Operator : SJ/JU
Sample : J1721-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

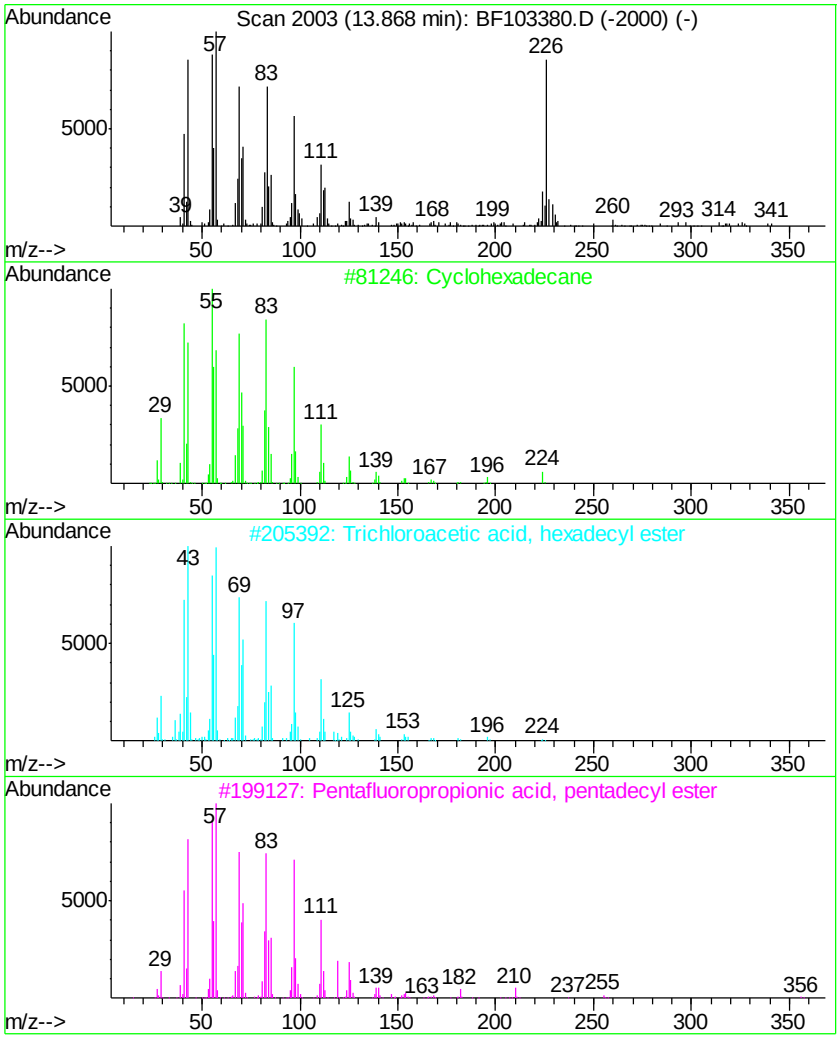
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

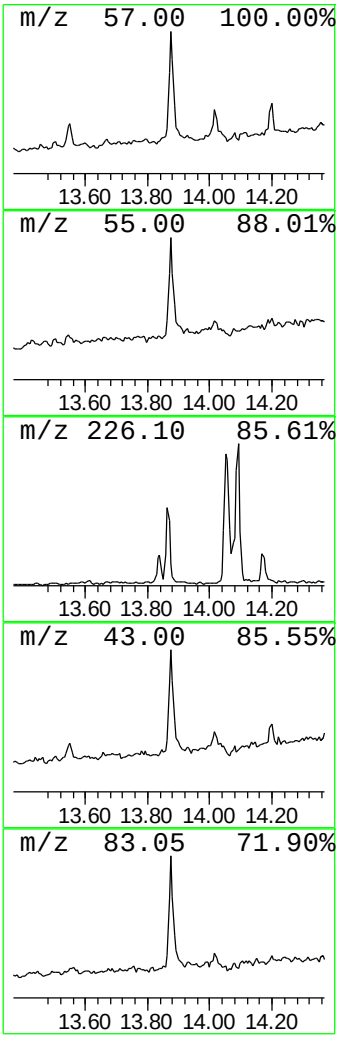
****

Peak Number 11 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.13 ng	437626	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF030218\
Data File : BF103380.D
Acq On : 2 Mar 2018 21:55
Operator : SJ/JU
Sample : J1721-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-46

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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
Butane, 2-methoxy...	2.13	6.0	ng	289883	1	6.87	959632	20.0
2-Pentanone, 4-hy...	5.11	2.5	ng	118120	1	6.87	959632	20.0
unknown6.65	6.65	64.1	ng	3073620	1	6.87	959632	20.0
Hexadecane	10.33	3.0	ng	167471	3	9.92	1113650	20.0
Pentadecane	10.80	4.6	ng	194710	4	11.41	854602	20.0
n-Hexadecanoic acid	11.92	3.4	ng	146066	4	11.41	854602	20.0
Phenanthrene, 1-m...	11.94	2.0	ng	86261	4	11.41	854602	20.0
4H-Cyclopenta[def...	12.03	2.9	ng	121985	4	11.41	854602	20.0
Phenanthrene, 2,5...	12.46	2.4	ng	103816	4	11.41	854602	20.0
Cyclohexadecane	13.87	8.1	ng	437626	5	14.06	1076240	20.0