LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103768.D
Acq On : 19 Mar 2018 20:57
Operator : JU/SJ
Sample : J1972-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

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-BF031518.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	2.334	35	42	48	rVB	166874	220571	4.42%	0.491%
2	5.234	531	535	548	rVB	185128	282716	5.67%	0.629%
3	5.604	592	598	601	rBV	4065001	4747496	95.22%	10.560%
4	5.922	648	652	660	rVB	84590	85595	1.72%	0.190%
5	6.604	761	768	772	rVB2	3664318	4985672	100.00%	11.090%
6	6.745	787	792	795	rBV	4205163	4756977	95.41%	10.581%
7	6.975	827	831	834	rBV	1255609	1028289	20.62%	2.287%
8	7.134	853	858	861	rBV	3884135	3714962	74.51%	8.263%
9	7.539	921	927	930	rBV	2985691	3156258	63.31%	7.021%
10	7.598	933	937	941	rVB	70306	66106	1.33%	0.147%
11	8.257	1045	1049	1052	rBV	1553016	1392285	27.93%	3.097%
12	8.851	1144	1150	1155	rBV2	139400	147596	2.96%	0.328%
13	9.333	1225	1232	1235	rBV	4702908	4720901	94.69%	10.501%
14	9.716	1294	1297	1301	rBV	871602	722034	14.48%	1.606%
15	9.786	1306	1309	1311	rBV	67555	62298	1.25%	0.139%
16	9.927	1328	1333	1336	rBV	132708	98832	1.98%	0.220%
17	10.016	1344	1348	1351	rBV	1719974	1471514	29.51%	3.273%
18	10.192	1375	1378	1380	rBV	159592	141607	2.84%	0.315%
19	10.427	1416	1418	1421	rVB	157823	120746	2.42%	0.269%
20	10.651	1448	1456	1458	rBV	54095	74085	1.49%	0.165%
21	10.727	1462	1469	1474	rVB2	105851	179077	3.59%	0.398%
22	10.810	1478	1483	1486	rBV	2815138	2872818	57.62%	6.390%
23	10.904	1496	1499	1509	rVB	144341	165490	3.32%	0.368%
24	11.057	1521	1525	1529	rVB2	41537	54594	1.10%	0.121%
25	11.351	1572	1575	1578	rBV	91625	76017	1.52%	0.169%
26	11.510	1597	1602	1604	rBV	1465813	1369027	27.46%	3.045%
27	11.527	1604	1605	1610	rVB	222957	188821	3.79%	0.420%
28	12.016	1684	1688	1690	rBV2	256871	235666	4.73%	0.524%
29	12.121	1701	1706	1708	rBV2	63492	71876	1.44%	0.160%
30	12.339	1739	1743	1746	rVB3	56706	59870	1.20%	0.133%
31	12.557	1777	1780	1783	rBV2	45055	53147	1.07%	0.118%
32	12.721	1805	1808	1812	rBV	466974	409308	8.21%	0.910%
33	12.804	1817	1822	1827	rBV4	42513	87482	1.75%	0.195%
34	12.898	1833	1838	1841	rBV4	41707	52395	1.05%	0.117%

LSC Area Percent Report

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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

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-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.957	1841	1848	1850	rBV	362872	396950	7.96%	0.883%
36	13.098	1865	1872	1875	rBV	3549040	3516866	70.54%	7.823%
37	13.280	1901	1903	1906	rVB	58226	52698	1.06%	0.117%
38	13.974	2018	2021	2024	rBV2	230474	201412	4.04%	0.448%
39	14.121	2043	2046	2048	rBV	80961	75521	1.51%	0.168%
40	14.157	2048	2052	2055	rVV2	1052688	1199221	24.05%	2.667%
41	14.186	2055	2057	2062	rVB	181931	172765	3.47%	0.384%
42	15.239	2233	2236	2239	rBV	155617	219608	4.40%	0.488%
43	15.321	2248	2250	2254	rVB	64202	61228	1.23%	0.136%
44	15.562	2289	2291	2297	rVB	99994	124508	2.50%	0.277%
45	15.633	2299	2303	2309	rVB	135281	185109	3.71%	0.412%
46	15.704	2310	2315	2319	rBV	664158	879719	17.64%	1.957%

Sum of corrected areas: 44957733

LSC Report - Integrated Chromatogram

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Sample : J1972-06
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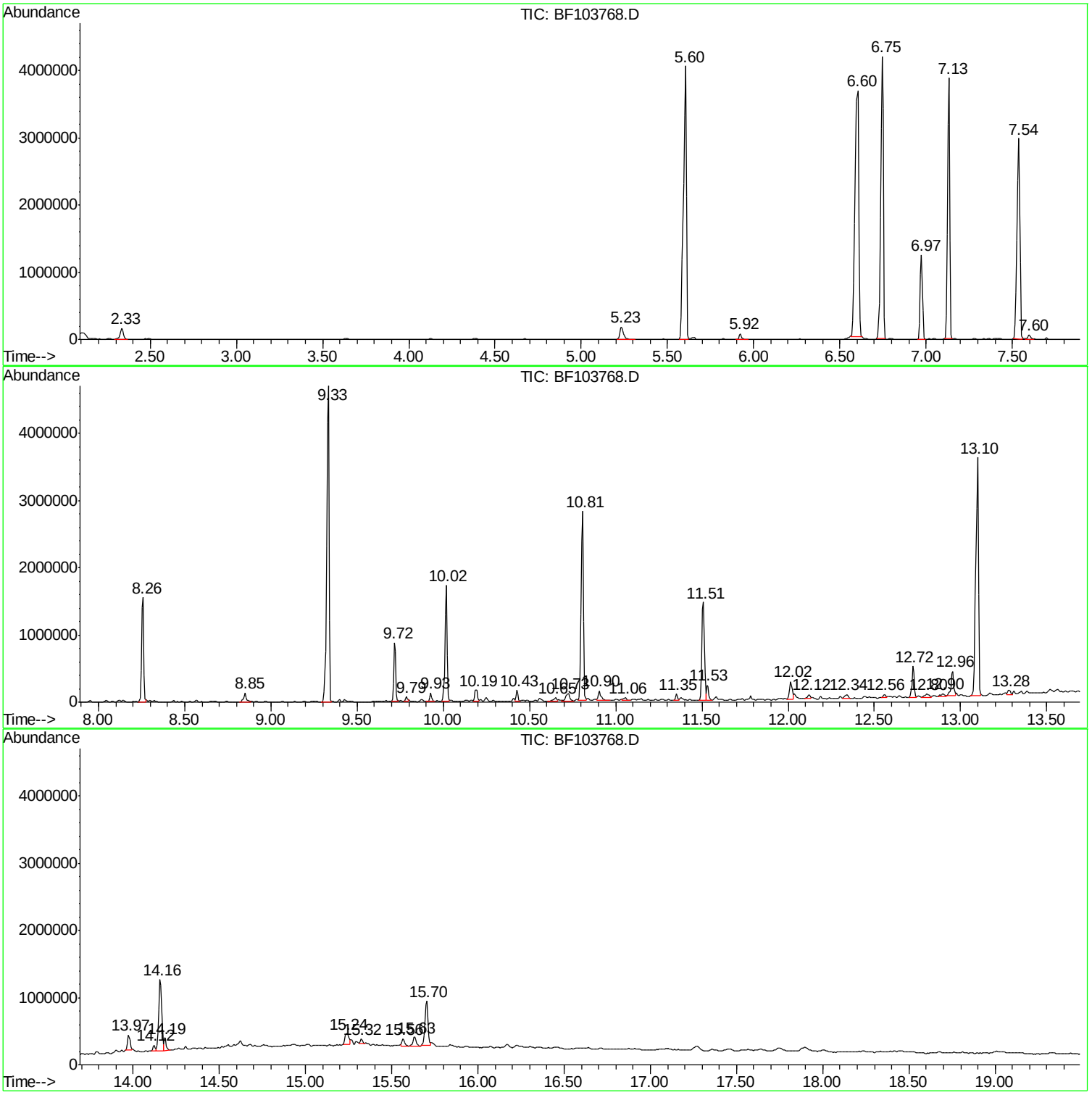
Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103768.D
Acq On : 19 Mar 2018 20:57
Operator : JU/SJ
Sample : J1972-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

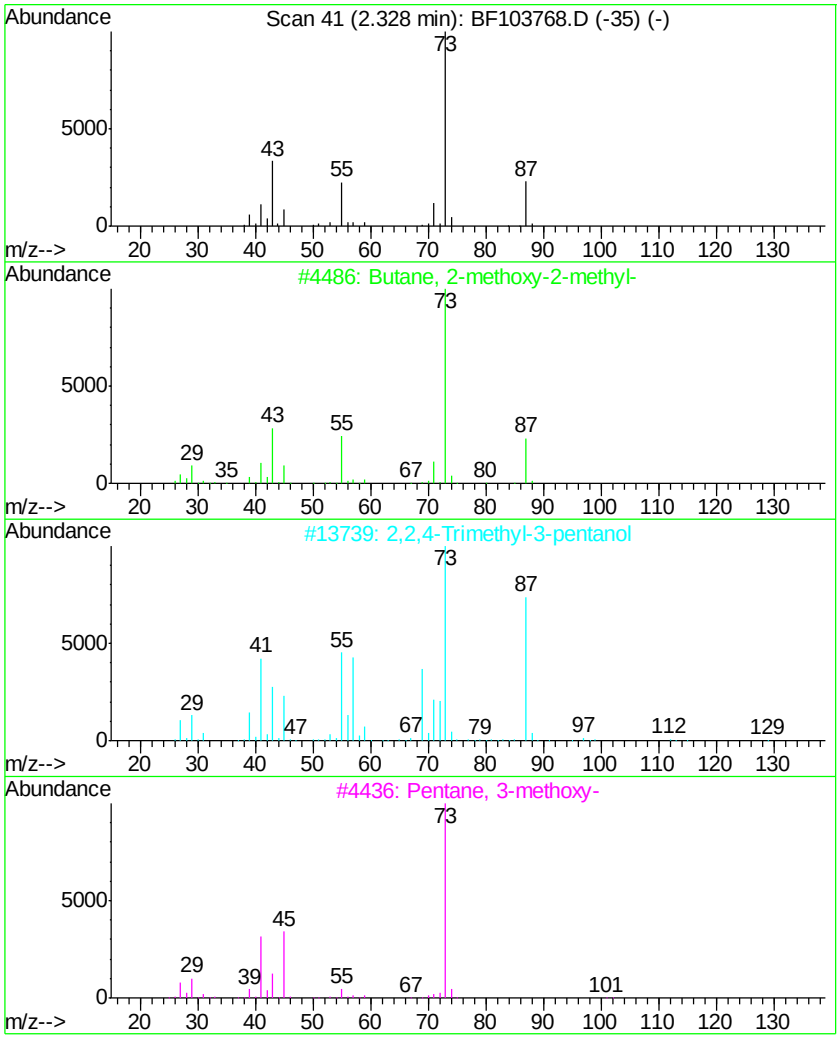
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

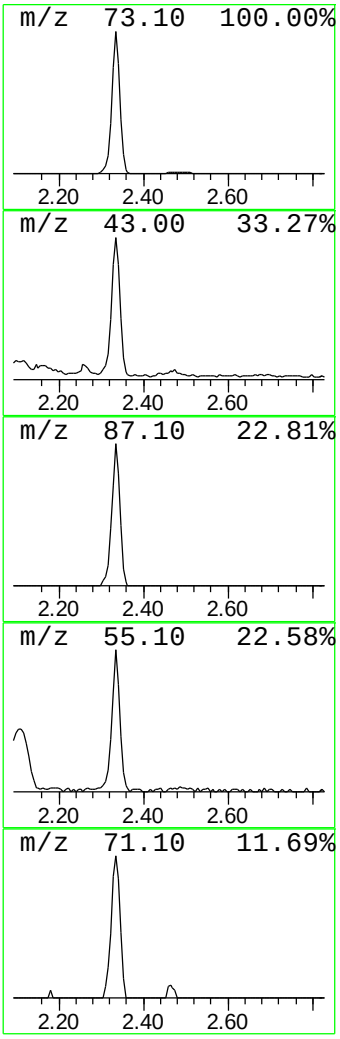
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	4.29 ng	220571	1,4-Dichlorobenzene-d4	6.97

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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Operator : JU/SJ
Sample : J1972-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

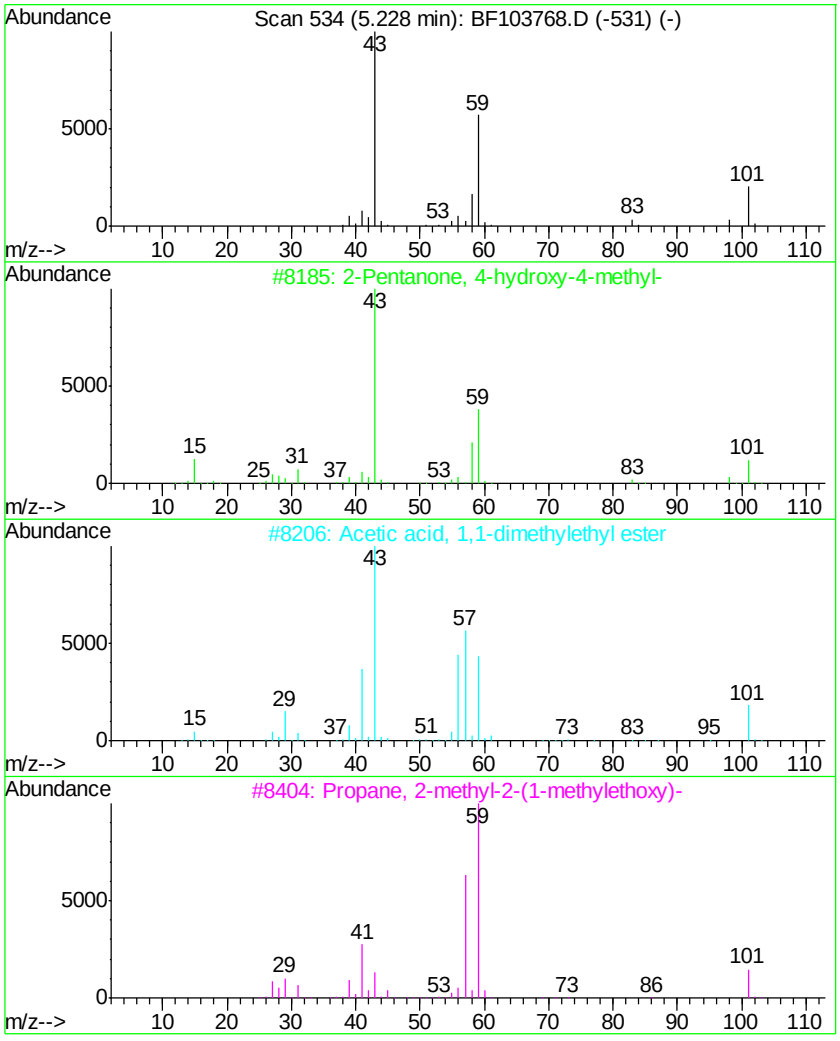
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

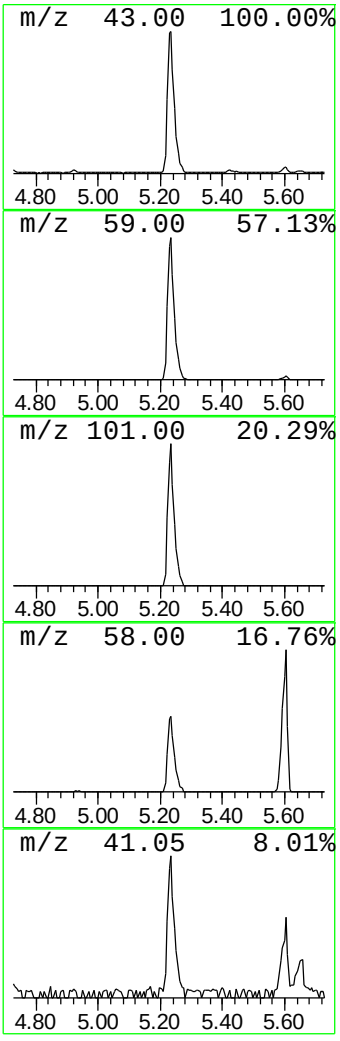
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	5.50 ng	282716	1,4-Dichlorobenzene-d4	6.97

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	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Sample : J1972-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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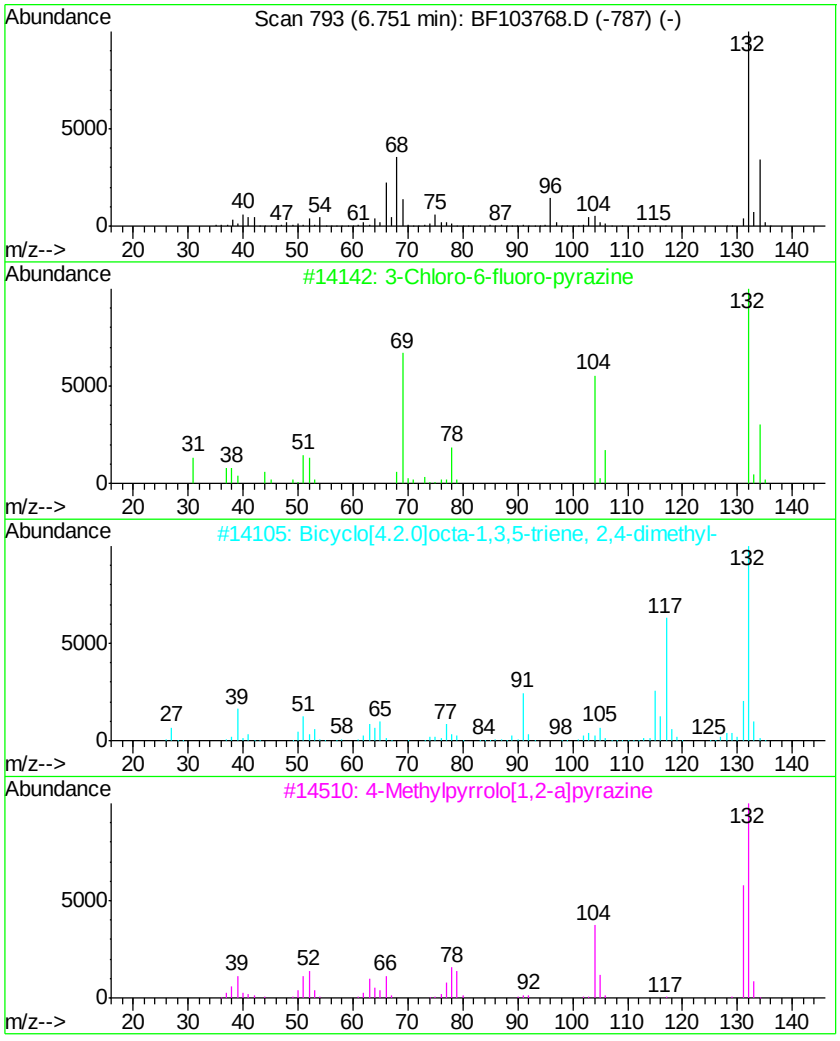
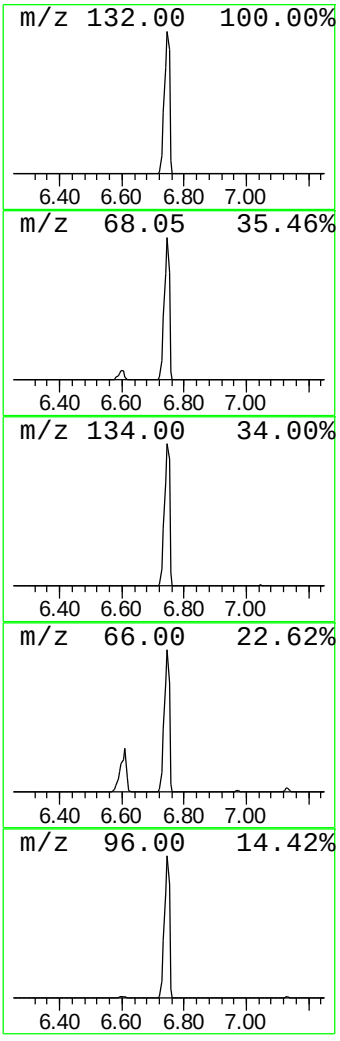
Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	92.52 ng	4756980	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : J1972-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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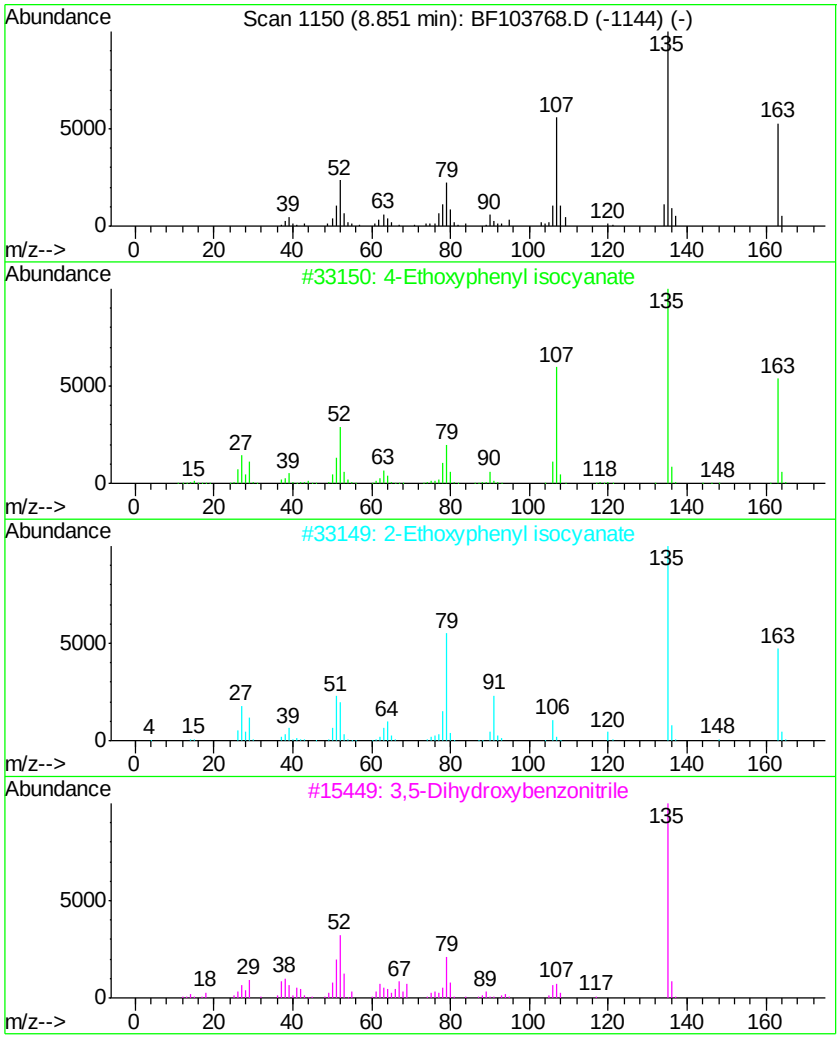
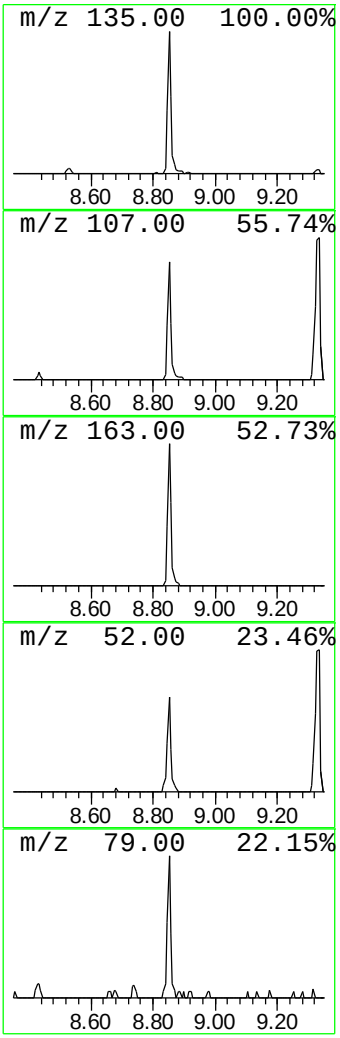
Peak Number 5 4-Ethoxyphenyl isocyanate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.85	2.12 ng	147596	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Ethoxyphenyl isocyanate	163	C9H9NO2	032459-62-4	96
2	2-Ethoxyphenyl isocyanate	163	C9H9NO2	005395-71-1	68
3	3,5-Dihydroxybenzonitrile	135	C7H5NO2	019179-36-3	58
4	2H-1,4-Benzoxazine-2,3(4H)-dione	163	C8H5NO3	003597-63-5	53
5	Pyrrolo(2,3-d)pyrimidin-4-one	135	C6H5N3O	003680-71-5	50





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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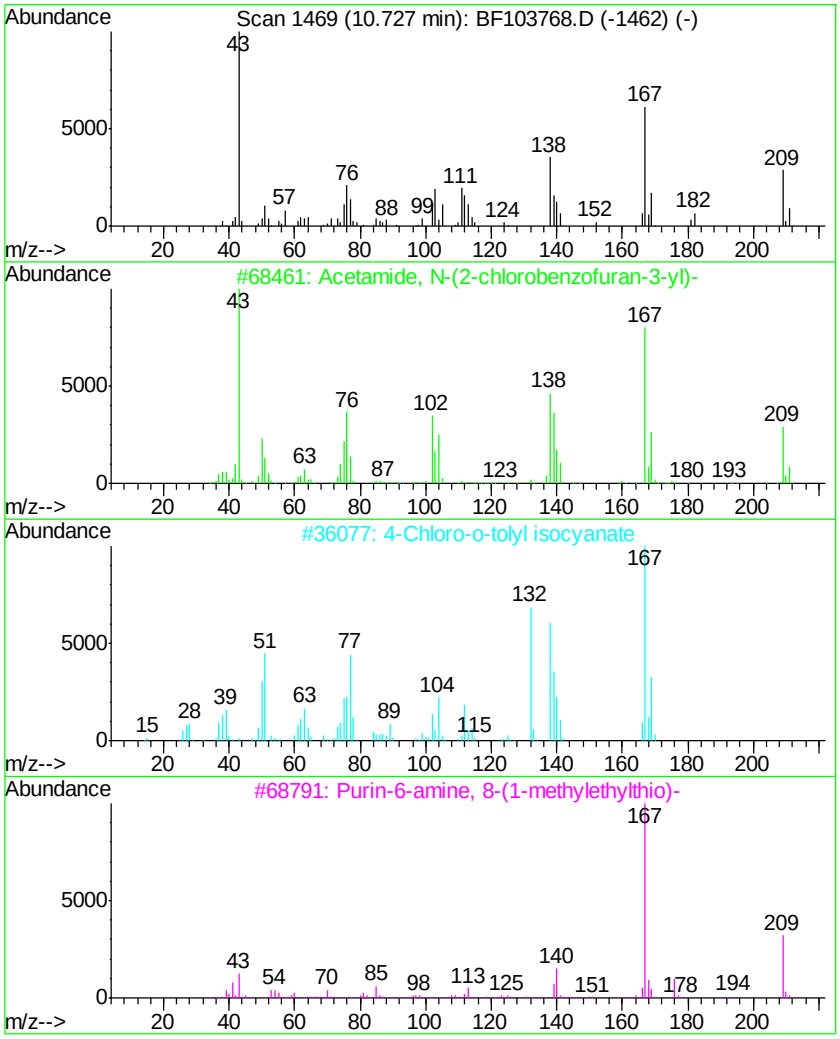
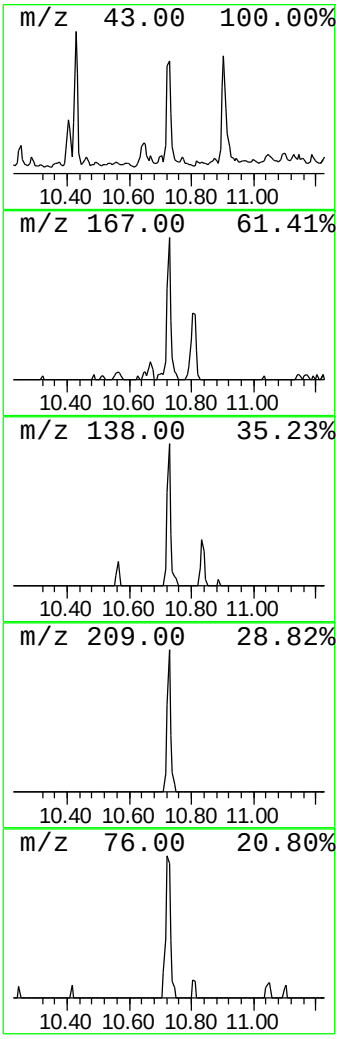
****

Peak Number 6 Acetamide, N-(2-chlorobenzo... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.43 ng	179077	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2-chlorobenzofuran...	209	C10H8ClNO2	067382-11-0	80
2	4-Chloro-o-tolyl isocyanate	167	C8H6ClNO	037408-18-7	49
3	Purin-6-amine, 8-(1-methylethylt...	209	C8H11N5S	330982-99-5	38
4	Indol-2-one, 5-chloro-1,3-dihydro-	167	C8H6ClNO	017630-75-0	37
5	1H-Indole-2,3-dione, 7-chloro-5-...	195	C9H6ClNO2	155184-80-8	37





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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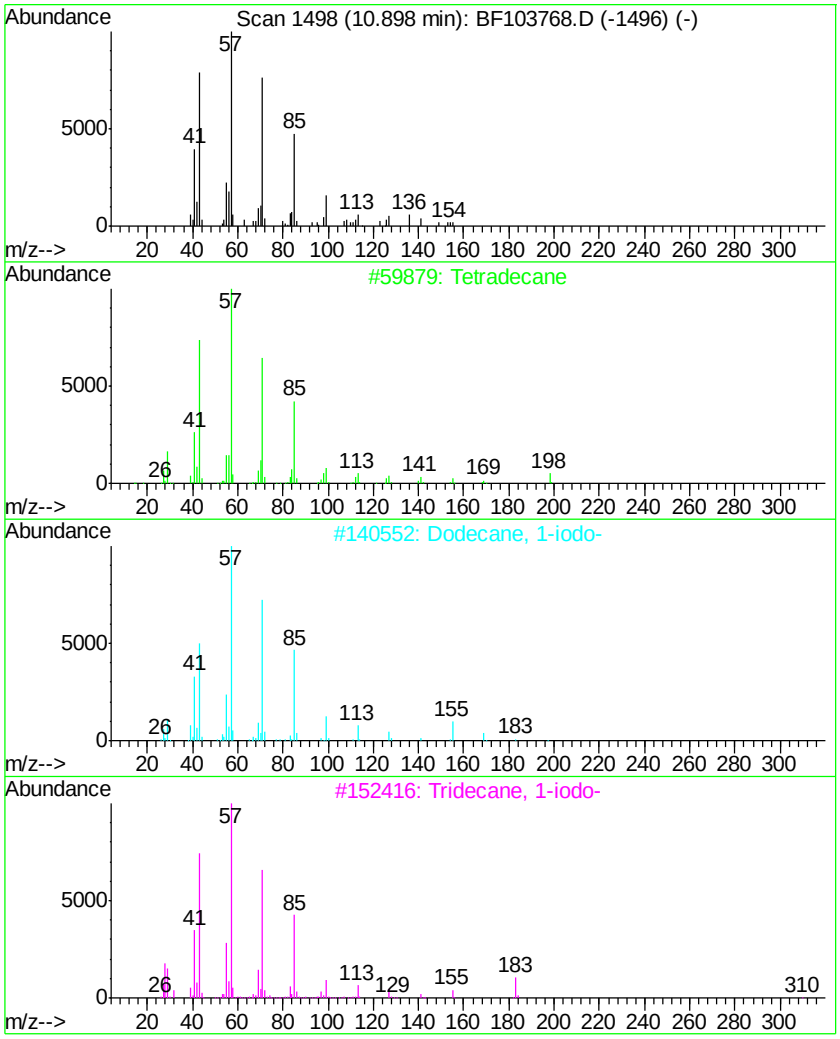
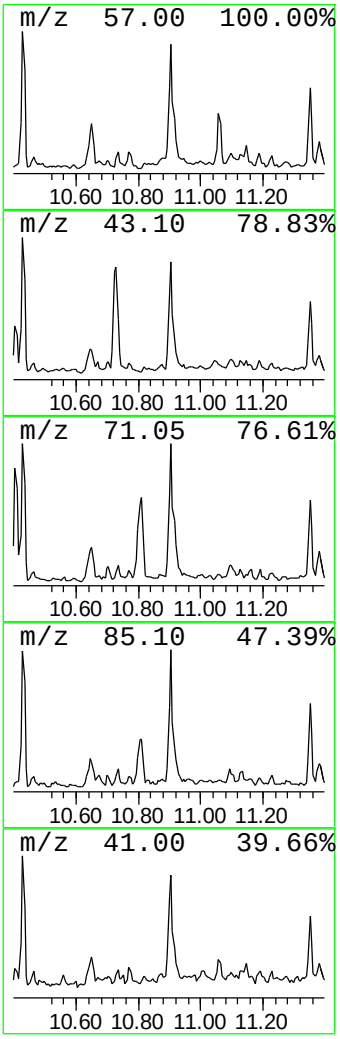
Peak Number 7 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.42 ng	165490	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72





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Instrument : BNA_F
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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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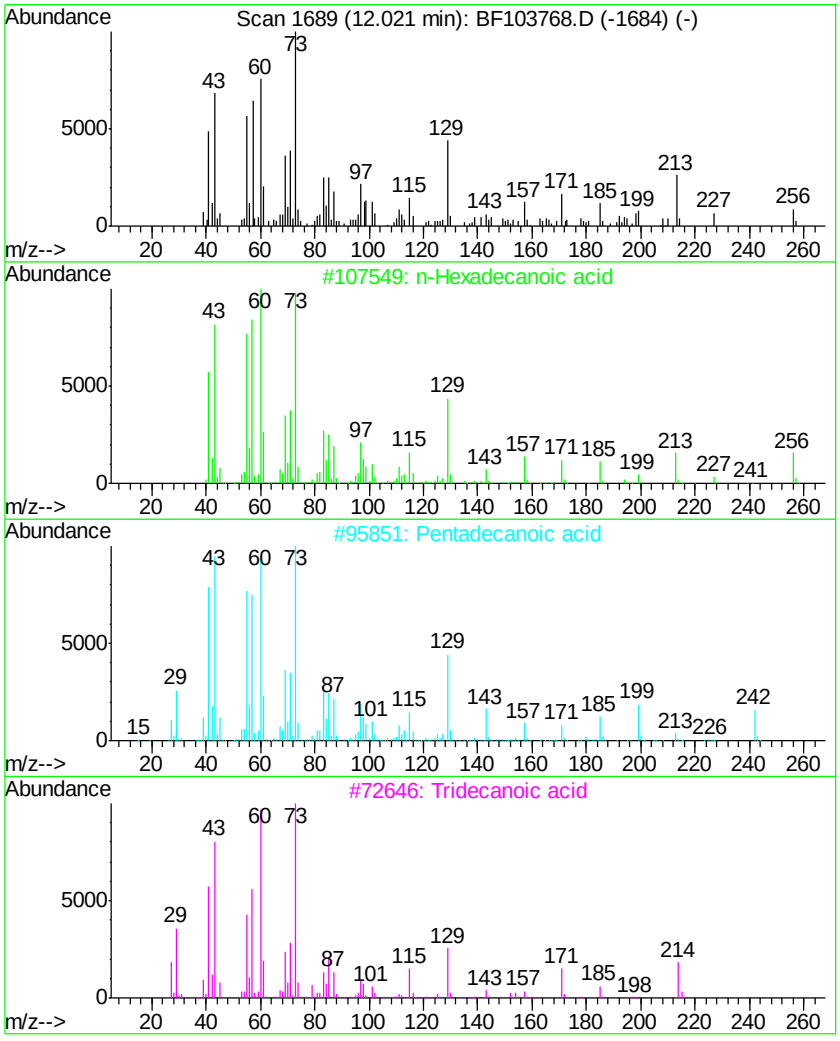
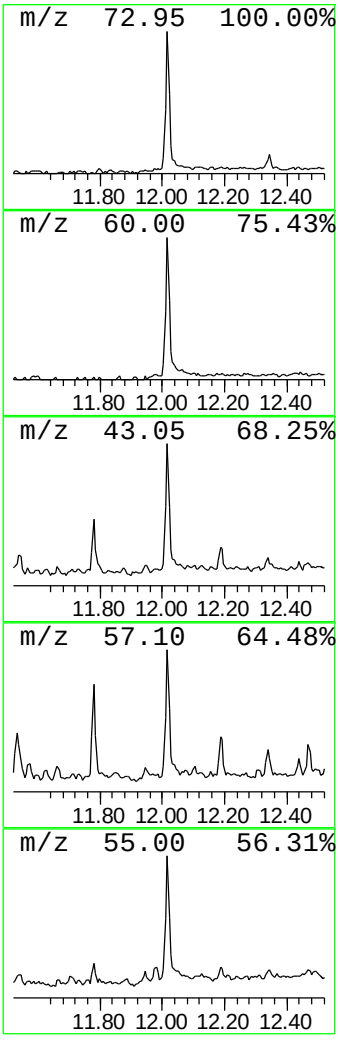
Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.44 ng	235666	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tetradecane	198	C14H30	000629-59-4	56





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Sample : J1972-06
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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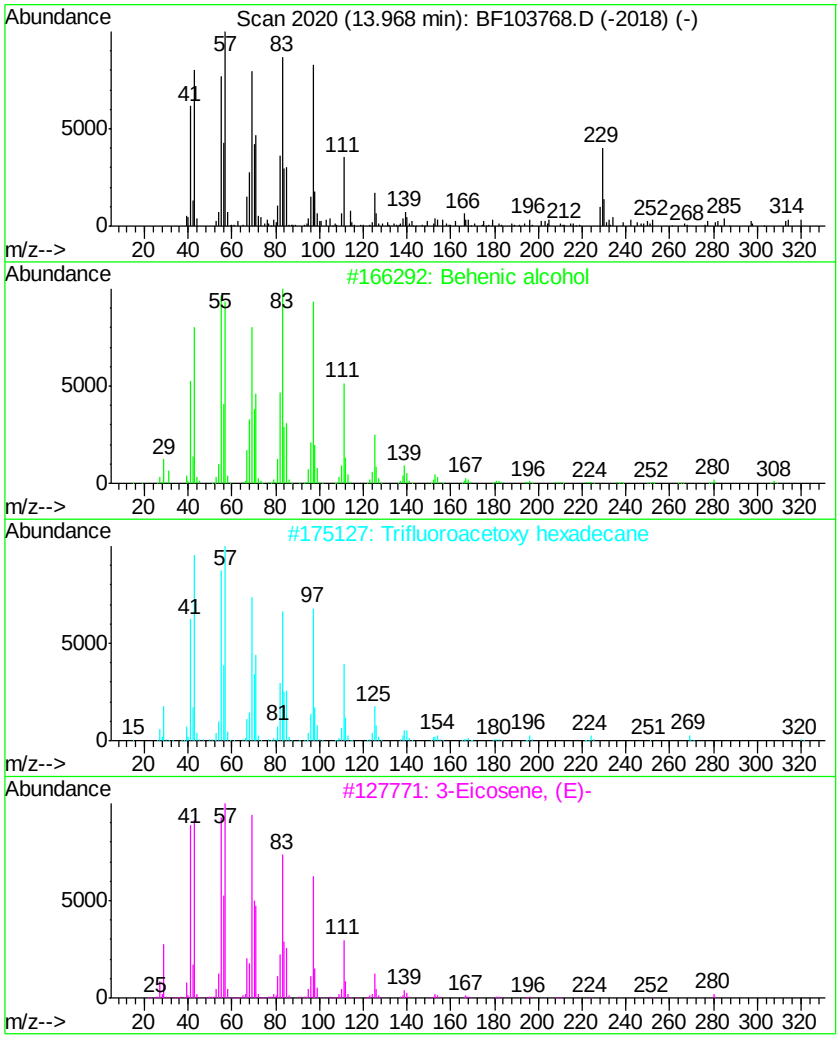
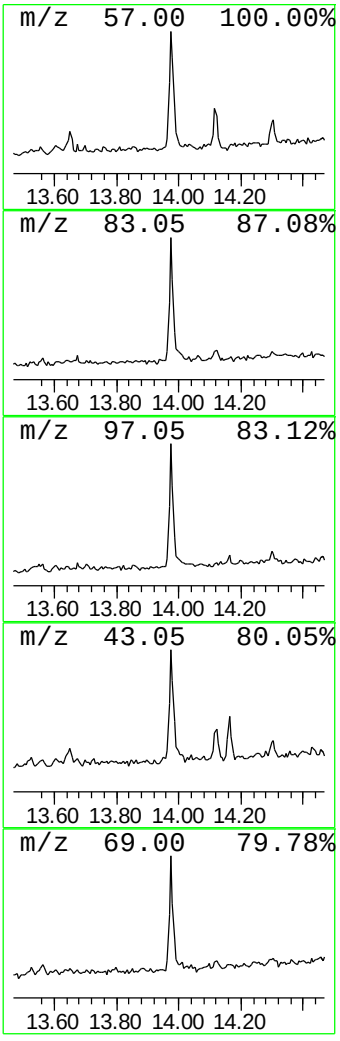
Peak Number 9 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.36 ng	201412	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103768.D
Acq On : 19 Mar 2018 20:57
Operator : JU/SJ
Sample : J1972-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

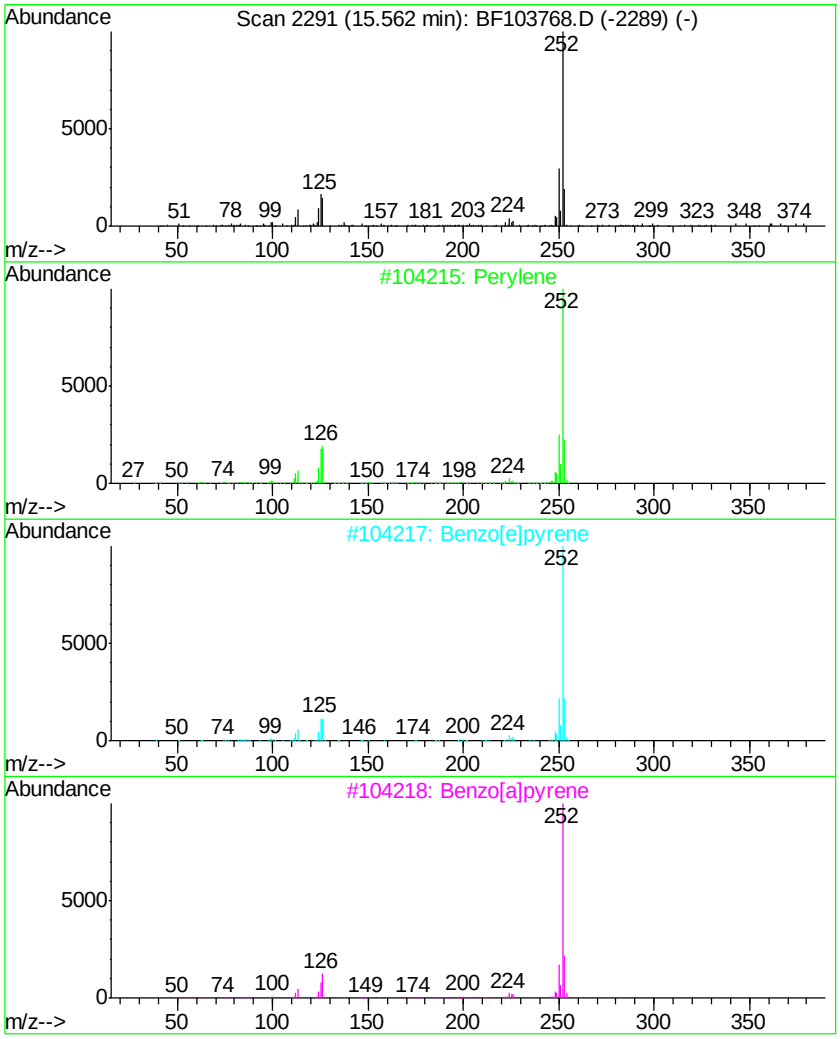
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

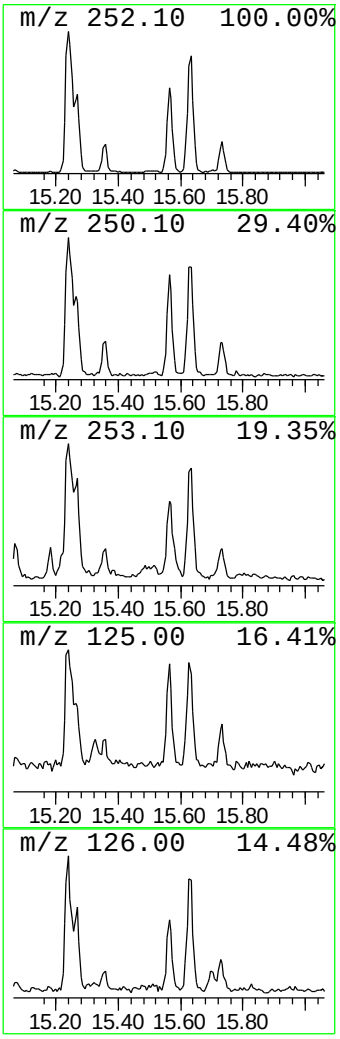
****

Peak Number 10 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	2.83 ng	124508	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	93
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	90
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103768.D
Acq On : 19 Mar 2018 20:57
Operator : JU/SJ
Sample : J1972-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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...	2.33	4.3	ng	220571	1	6.97	1028290	20.0
2-Pentanone, 4-hy...	5.23	5.5	ng	282716	1	6.97	1028290	20.0
unknown6.75	6.75	92.5	ng	4756980	1	6.97	1028290	20.0
4-Ethoxyphenyl is...	8.85	2.1	ng	147596	2	8.26	1392290	20.0
Acetamide, N-(2-c...	10.73	2.4	ng	179077	3	10.02	1471510	20.0
Tetradecane	10.90	2.4	ng	165490	4	11.51	1369030	20.0
n-Hexadecanoic acid	12.02	3.4	ng	235666	4	11.51	1369030	20.0
Behenic alcohol	13.97	3.4	ng	201412	5	14.16	1199220	20.0
Perylene	15.56	2.8	ng	124508	6	15.70	879719	20.0