LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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	5.104	510	513	526	rBV	37215	92052	2.49%	0.231%
2	5.487	575	578	613	rBV	1569991	3530183	95.43%	8.864%
3	6.498	747	750	769	rBV	1877244	3504288	94.73%	8.799%
4	6.628	769	772	798	rVB	2608218	3679140	99.46%	9.238%
5	6.857	808	811	833	rVB	452508	831720	22.48%	2.088%
6	7.010	833	837	862	rBV	2154538	2658567	71.87%	6.675%
7	7.428	904	908	932	rBV	1467692	2457709	66.44%	6.171%
8	8.139	1026	1029	1057	rBV	722418	1141253	30.85%	2.866%
9	9.075	1184	1188	1197	rVB	206840	208034	5.62%	0.522%
10	9.186	1204	1207	1208	rBV	197152	156610	4.23%	0.393%
11	9.210	1208	1211	1226	rVV	3092518	3699060	100.00%	9.288%
12	9.316	1226	1229	1238	rVV	115477	152069	4.11%	0.382%
13	9.392	1238	1242	1260	rVB	82560	236427	6.39%	0.594%
14	9.692	1289	1293	1301	rVB4	34803	45833	1.24%	0.115%
15	9.898	1324	1328	1342	rVB	1051586	1208358	32.67%	3.034%
16	10.280	1390	1393	1395	rBV	83406	66554	1.80%	0.167%
17	10.304	1395	1397	1401	rVB	45611	42707	1.15%	0.107%
18	10.516	1429	1433	1438	rVB2	32533	41095	1.11%	0.103%
19	10.698	1460	1464	1476	rBV	1637287	2342258	63.32%	5.881%
20	10.786	1477	1479	1483	rVB2	46733	53924	1.46%	0.135%
21	10.886	1492	1496	1500	rBV2	57250	65875	1.78%	0.165%
22	11.157	1539	1542	1548	rVB6	31006	42934	1.16%	0.108%
23	11.227	1551	1554	1557	rBV2	39764	57426	1.55%	0.144%
24	11.322	1567	1570	1574	rBV3	48225	39505	1.07%	0.099%
25	11.392	1579	1582	1586	rBV	1011562	1182997	31.98%	2.970%
26	11.486	1595	1598	1603	rVB2	28665	43139	1.17%	0.108%
27	11.539	1603	1607	1610	rBV	379435	339112	9.17%	0.851%
28	11.592	1613	1616	1622	rVB3	95890	128881	3.48%	0.324%
29	11.657	1624	1627	1629	rBV2	66259	54863	1.48%	0.138%
30	11.757	1643	1644	1650	rVB2	50495	42353	1.14%	0.106%
31	11.910	1666	1670	1672	rBV	998049	989501	26.75%	2.484%
32	11.939	1672	1675	1680	rVB	2101379	1919558	51.89%	4.820%
33	12.063	1694	1696	1699	rVB	82290	62340	1.69%	0.157%
34	12.145	1708	1710	1713	rVB2	68622	56661	1.53%	0.142%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

35	12.416	1753	1756	1759	rBV	110165	111574	3.02%	0.280%
36	12.451	1759	1762	1766	rVV	154068	129370	3.50%	0.325%
37	12.539	1774	1777	1779	rBV	65341	68029	1.84%	0.171%
38	12.616	1787	1790	1796	rVB	195011	237985	6.43%	0.598%
39	12.692	1800	1803	1807	rBV2	106987	110904	3.00%	0.278%
40	12.827	1823	1826	1828	rBV	298568	271337	7.34%	0.681%
41	12.851	1828	1830	1837	rVB	202237	203558	5.50%	0.511%
42	12.980	1847	1852	1862	rBV	2657362	2922271	79.00%	7.337%
43	13.180	1881	1886	1890	rVB	398610	486176	13.14%	1.221%
44	13.380	1918	1920	1923	rBV3	67045	81483	2.20%	0.205%
45	13.527	1941	1945	1949	rBV	314747	297006	8.03%	0.746%
46	13.851	1997	2000	2015	rVB	994282	1212193	32.77%	3.044%
47	13.992	2021	2024	2028	rVB	157634	134292	3.63%	0.337%
48	14.051	2030	2034	2044	rBV2	811393	1080948	29.22%	2.714%
49	14.174	2052	2055	2058	rBV	108267	104138	2.82%	0.261%
50	14.486	2105	2108	2112	rBV4	70275	120823	3.27%	0.303%
51	14.792	2157	2160	2165	rBV2	53988	64588	1.75%	0.162%
52	15.127	2213	2217	2220	rBV	128817	168018	4.54%	0.422%
53	15.510	2278	2282	2286	rBV3	97999	142349	3.85%	0.357%
54	15.562	2286	2291	2304	rVB	425141	707098	19.12%	1.775%

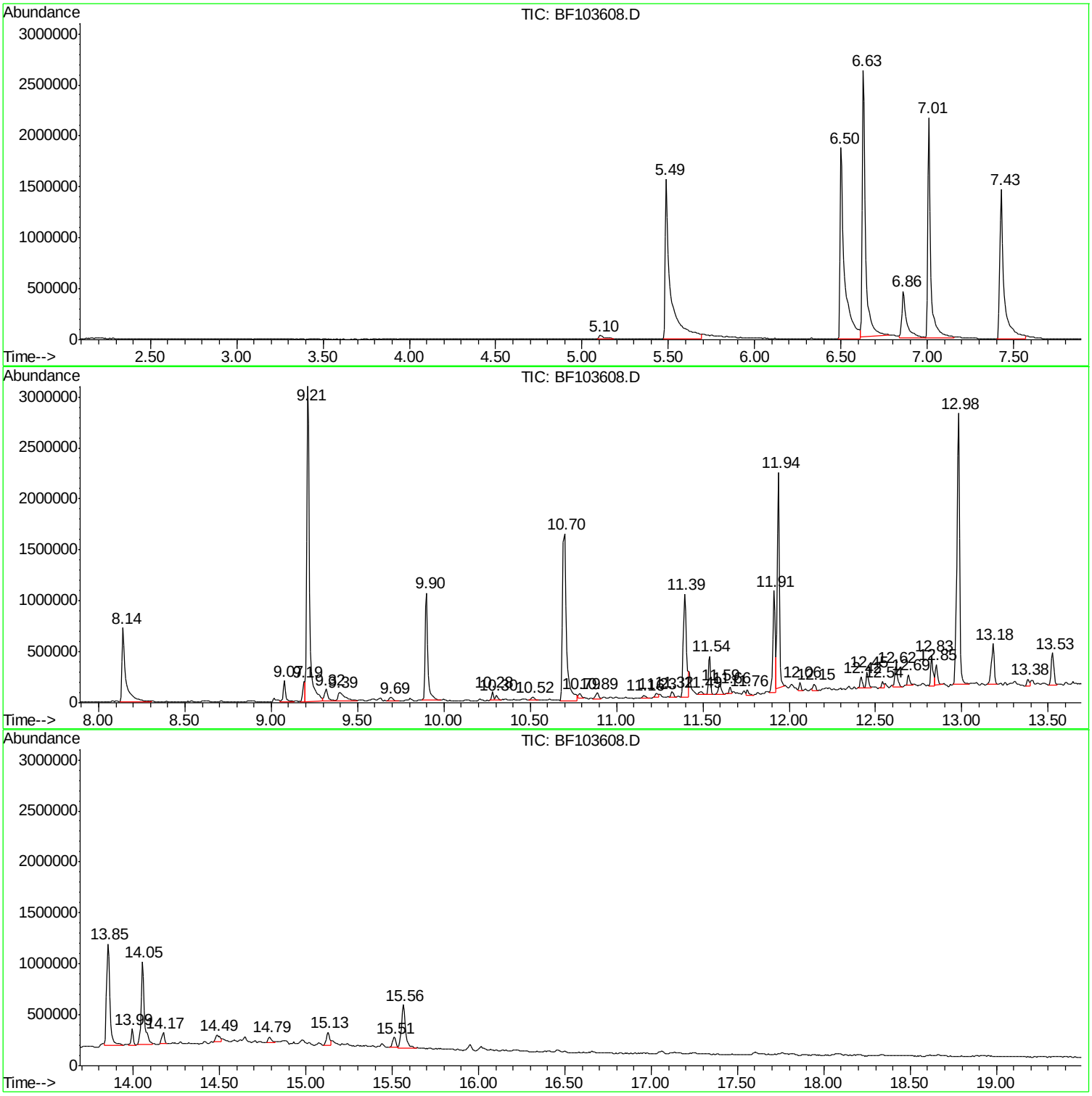
Sum of corrected areas: 39827126

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

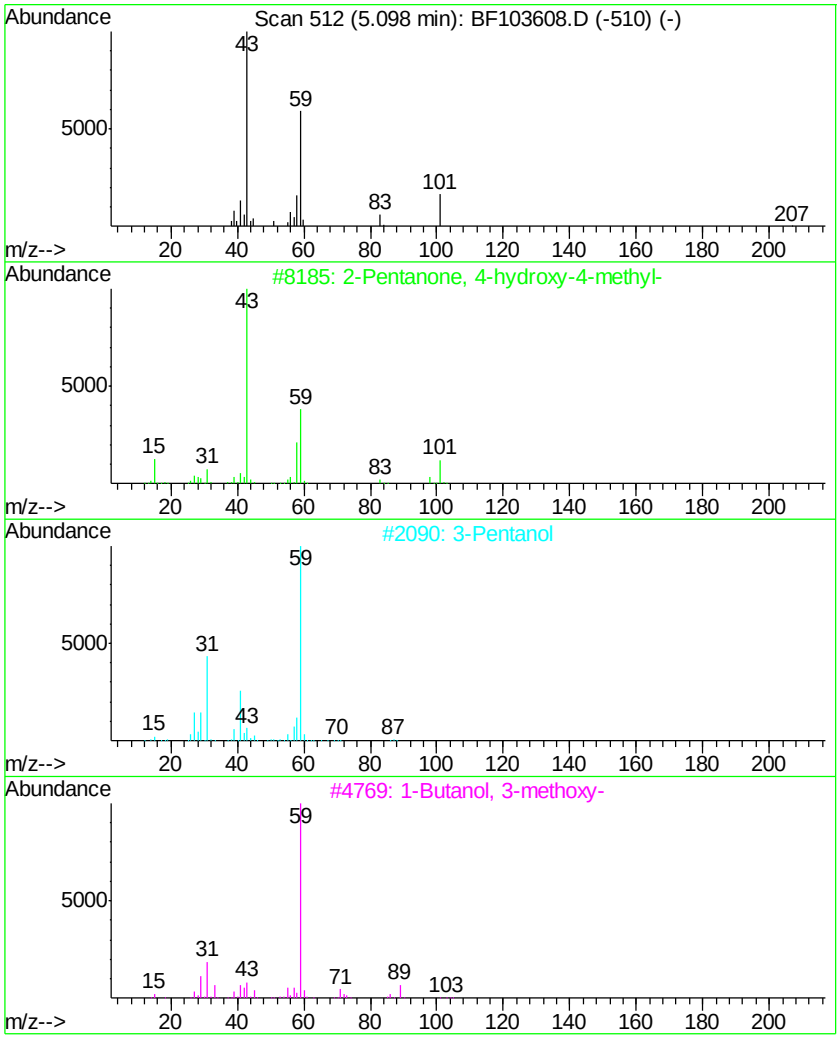
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

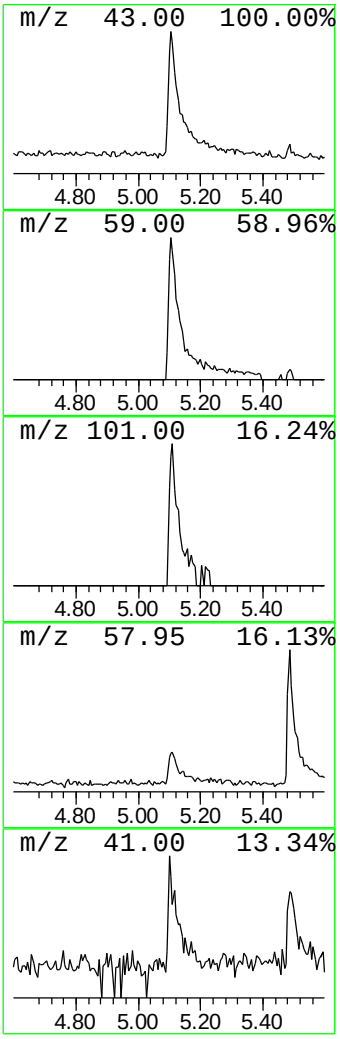
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.21 ng	92052	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	3-Pentanol	88	C5H12O	000584-02-1	38
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	37
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	1,2-Butanediol	90	C4H10O2	000584-03-2	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

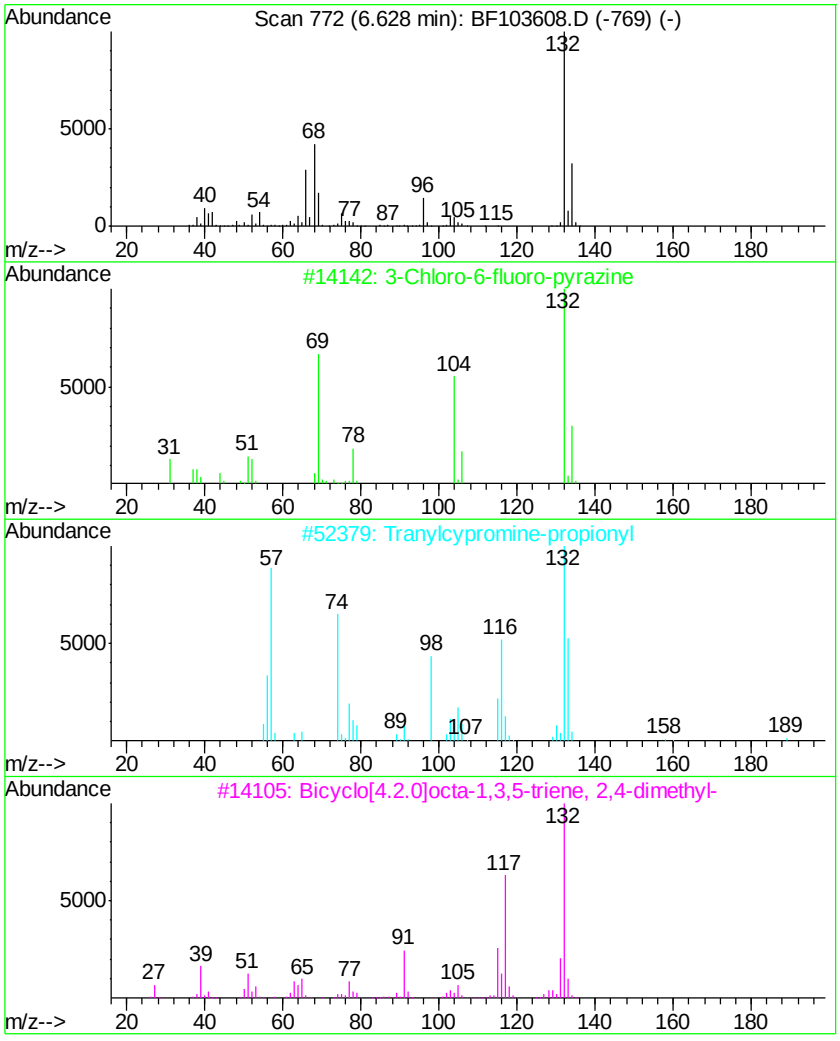
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

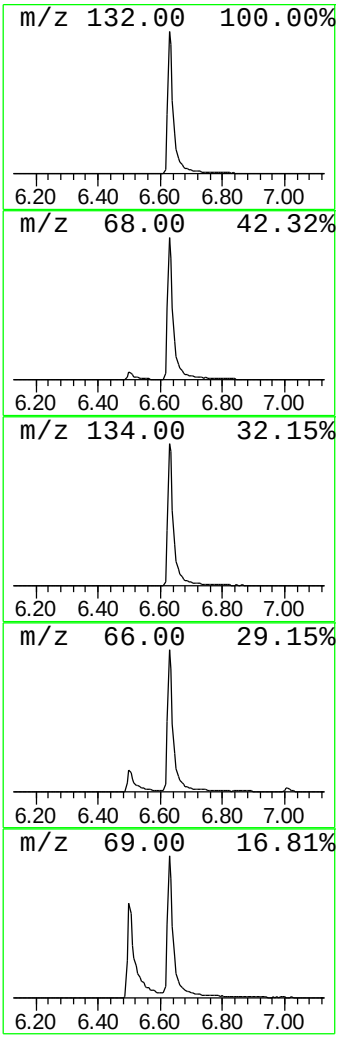
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	88.47 ng	3679140	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

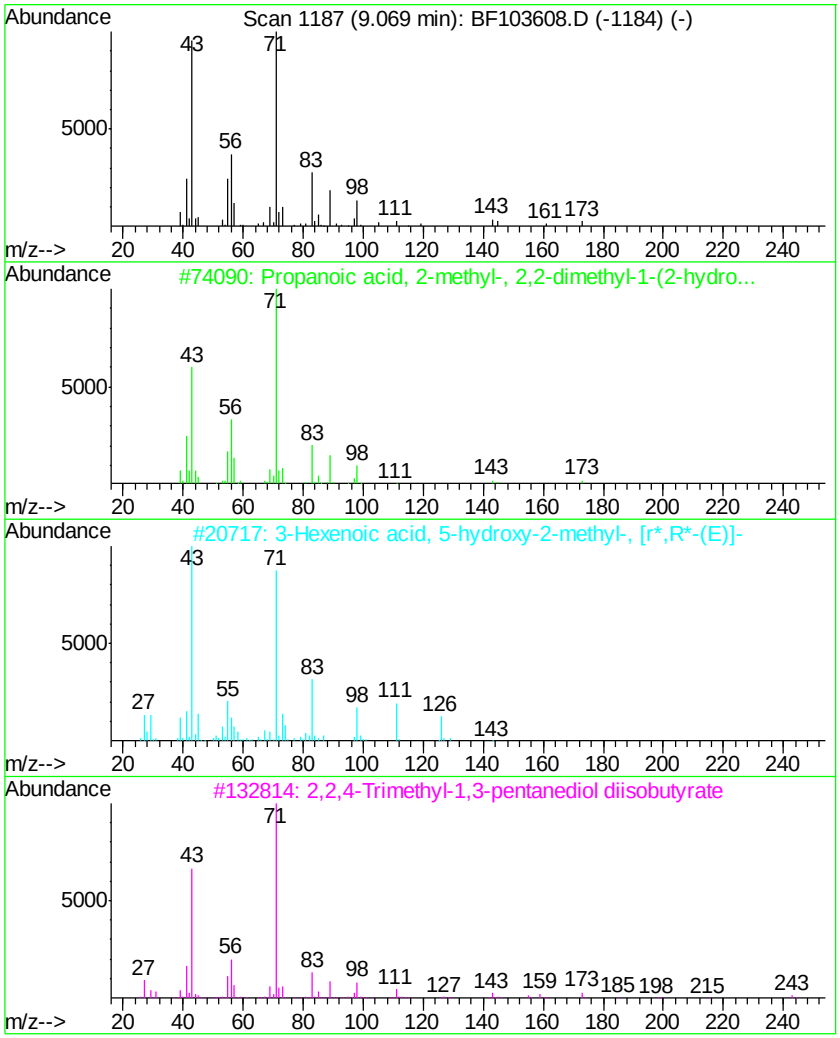
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

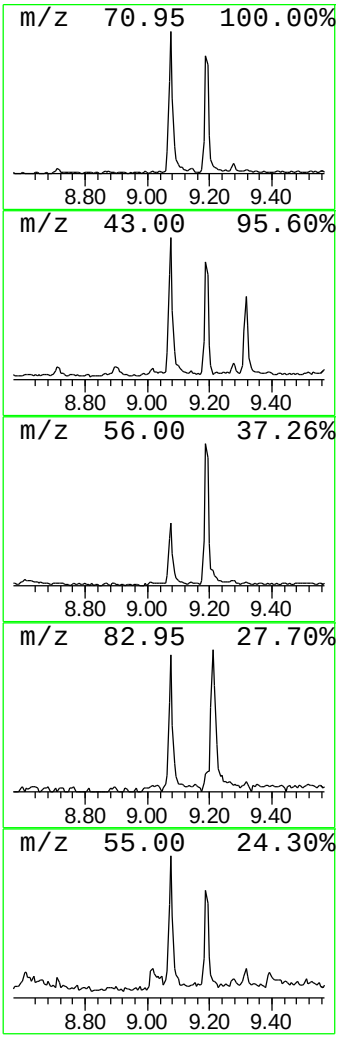
****

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.07	3.44 ng	208034	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	86
2	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	38
3	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	38
4	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	38
5	4,5-Octanedione	142	C8H14O2	005455-24-3	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

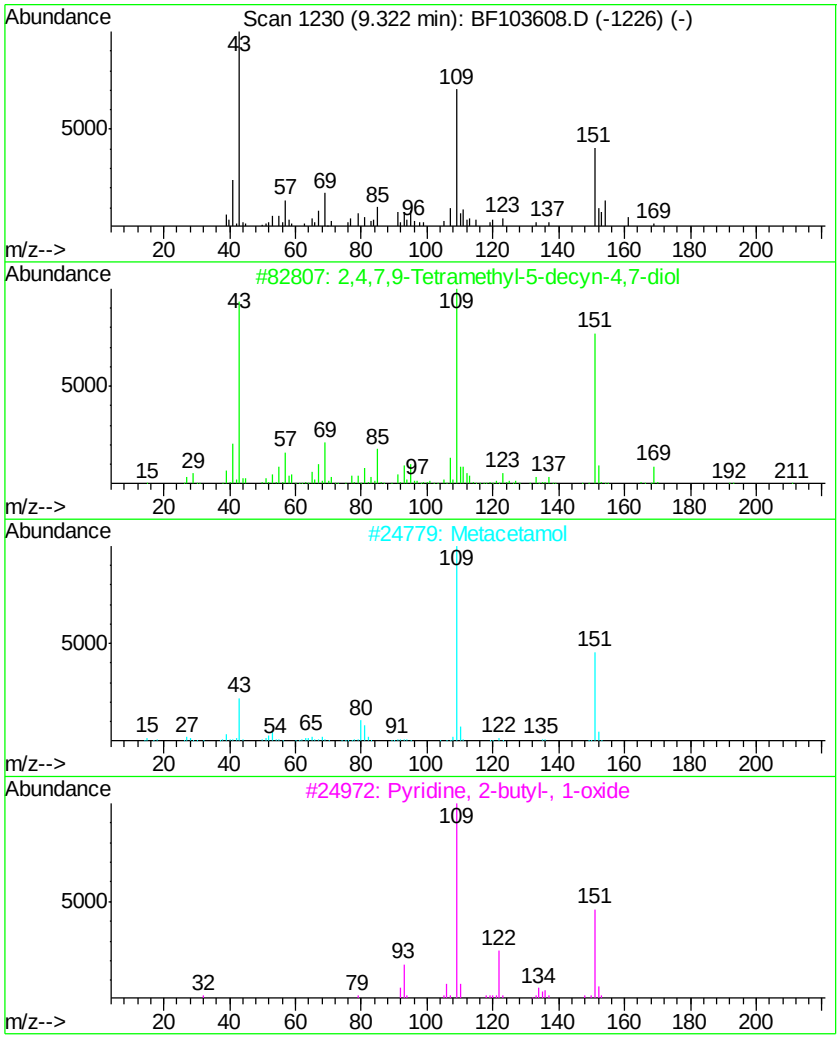
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

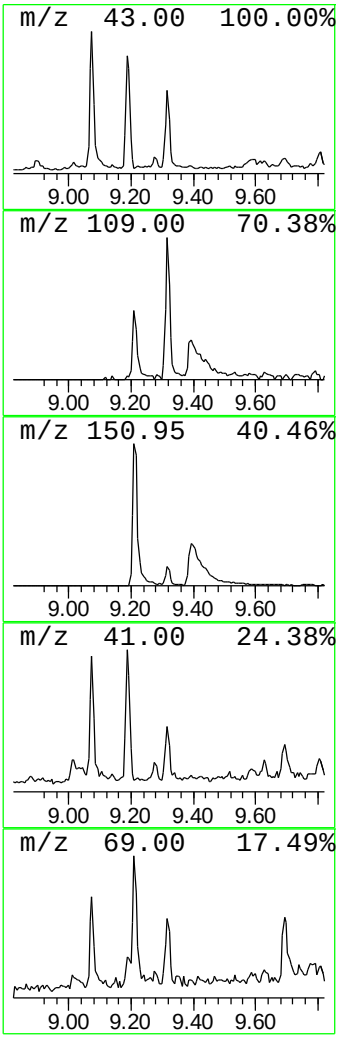
****

Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.32	2.52 ng	152069	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	80
2	Metacetamol	151	C8H9NO2	000621-42-1	58
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
4	Acetaminophen	151	C8H9NO2	000103-90-2	52
5	3-Pyridinemethanol, acetate	151	C8H9NO2	010072-09-0	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

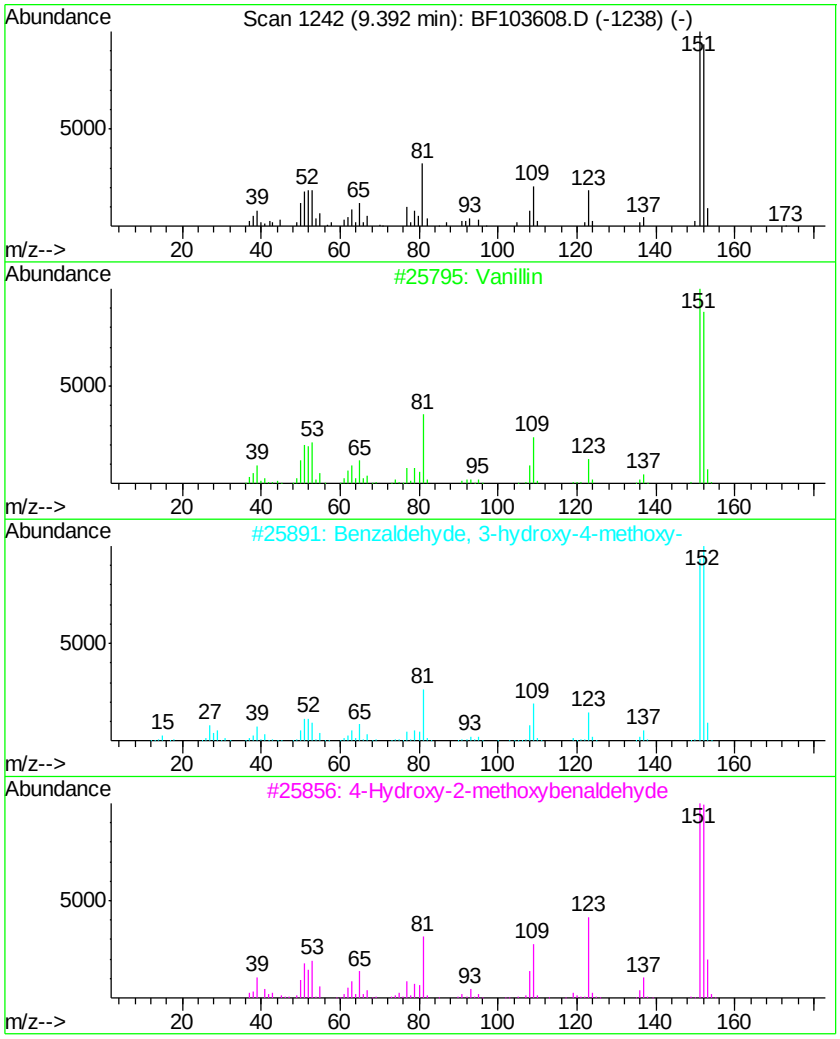
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

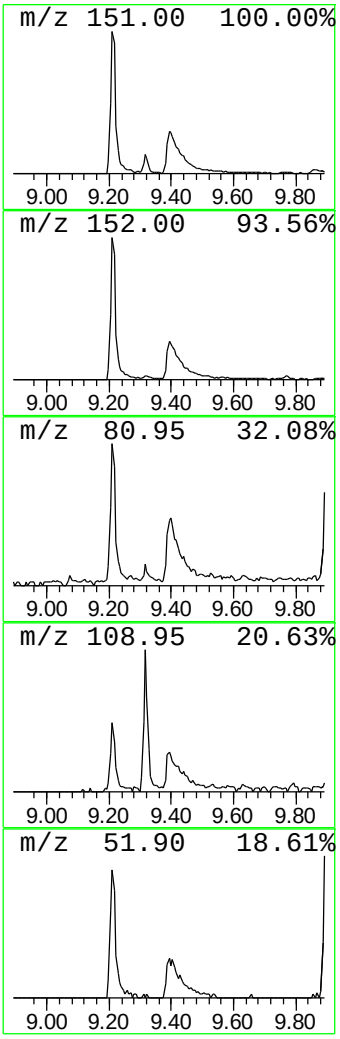
****

Peak Number 6 Vanillin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	3.91 ng	236427	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	97
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
3	4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	74
4	Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	72
5	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

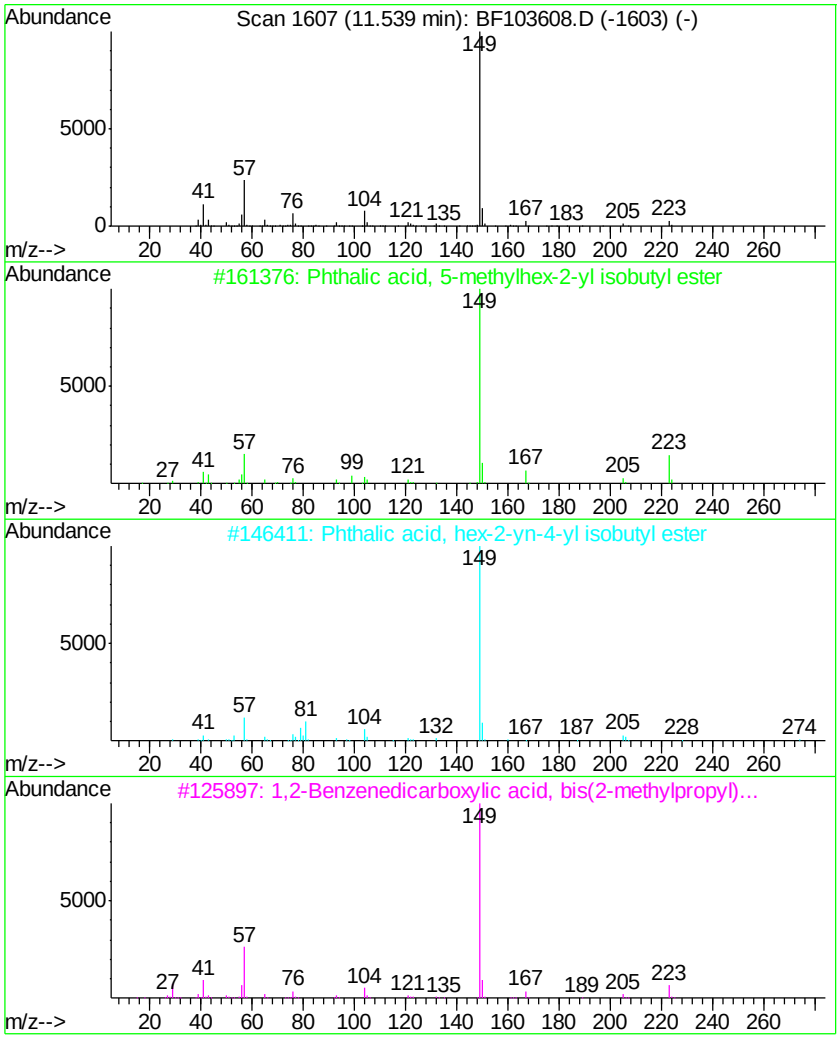
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

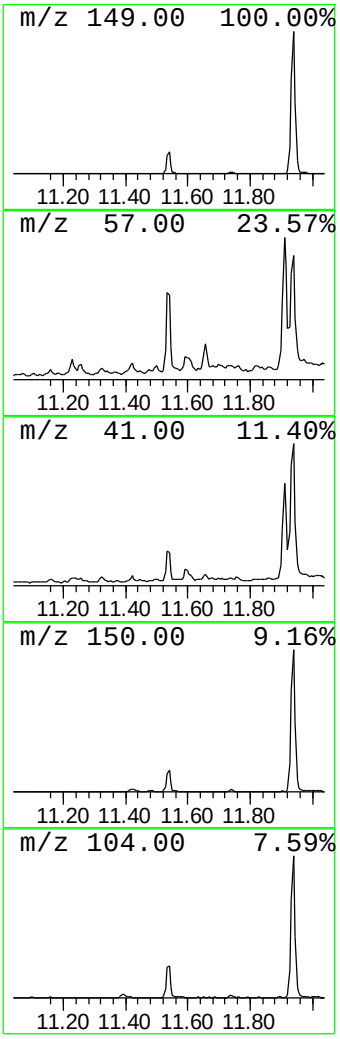
****

Peak Number 7 Phthalic acid, 5-methylhex-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	5.73 ng	339112	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 5-methylhex-2-yl ...	320	C19H28O4	1000371-09-1	86
2	Phthalic acid, hex-2-yn-4-yl iso...	302	C18H22O4	1000315-19-9	78
3	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	78
4	Phthalic acid, butyl hex-2-yn-4-...	302	C18H22O4	1000315-19-2	78
5	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-19-0	78





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Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

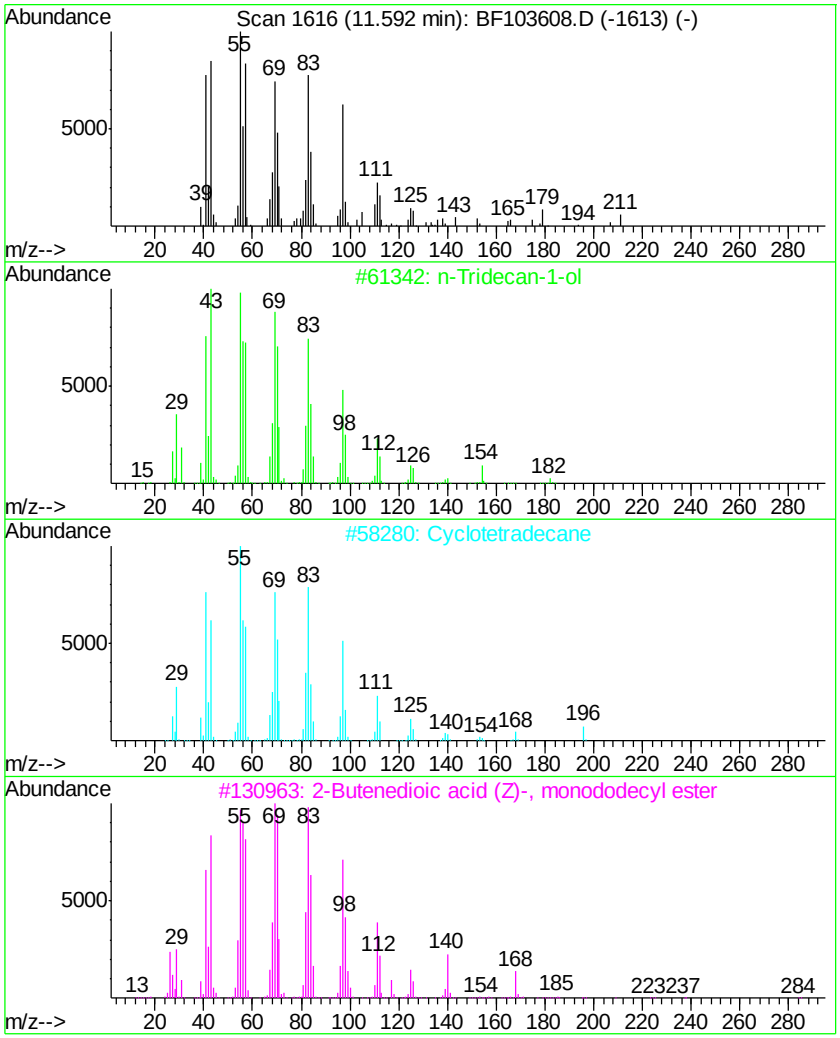
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

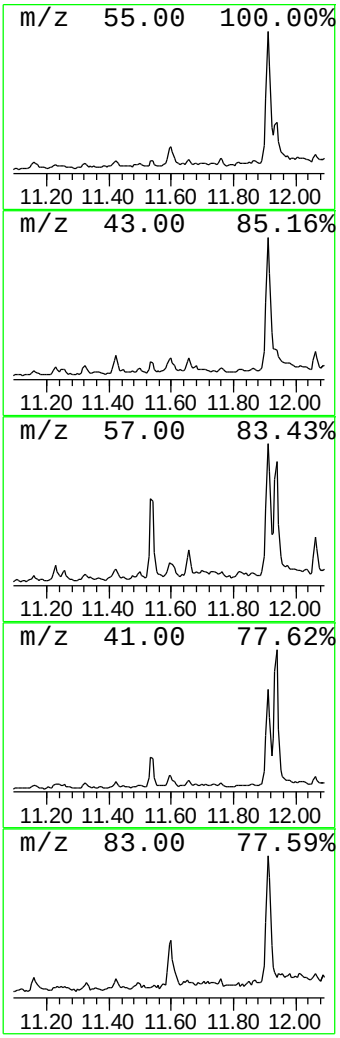
****

Peak Number 8 n-Tridecan-1-ol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.18 ng	128881	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tridecan-1-ol	200	C13H28O	000112-70-9	87
2	Cyclotetradecane	196	C14H28	000295-17-0	80
3	2-Butenedioic acid (Z)-, monodod...	284	C16H28O4	002424-61-5	74
4	Pentafluoropropionic acid, decyl...	304	C13H21F5O2	959000-65-8	64
5	Decyl trifluoroacetate	254	C12H21F3O2	000333-88-0	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103608.D
Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

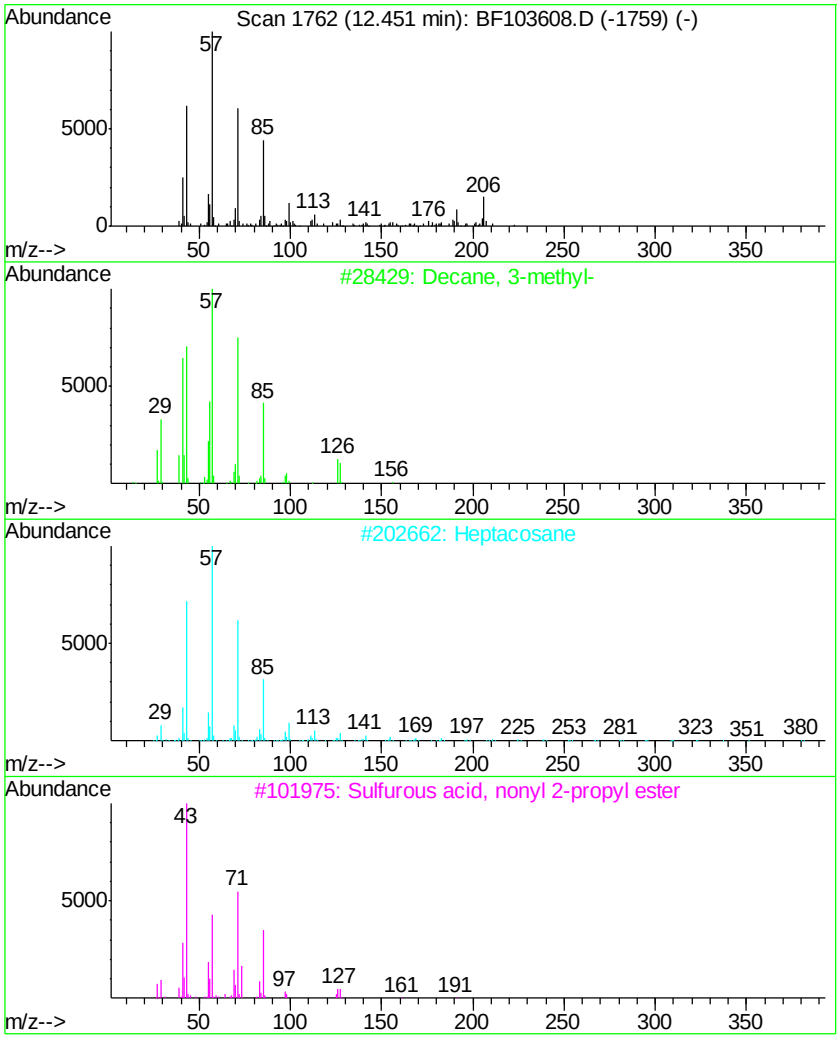
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

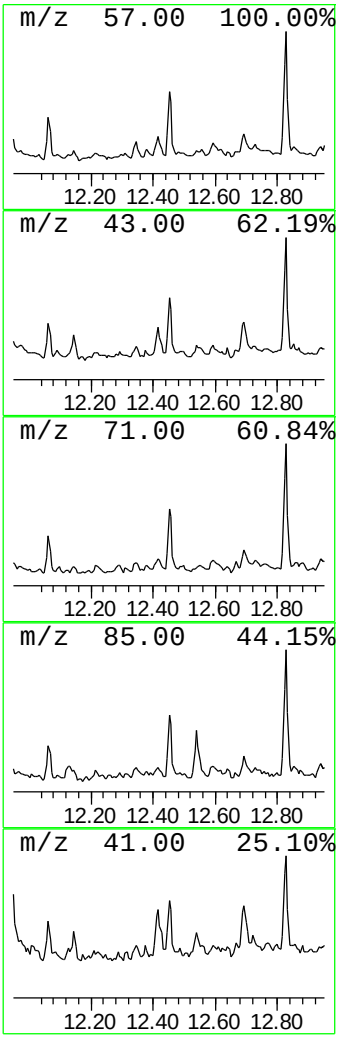
****

Peak Number 9 Decane, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	2.19 ng	129370	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-methyl-	156	C11H24	013151-34-3	64
2	Heptacosane	380	C27H56	000593-49-7	50
3	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	47
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	46
5	S-Butyl n-hexyl disulfide	206	C10H22S2	169611-28-3	45





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Acq On : 13 Mar 2018 17:01
Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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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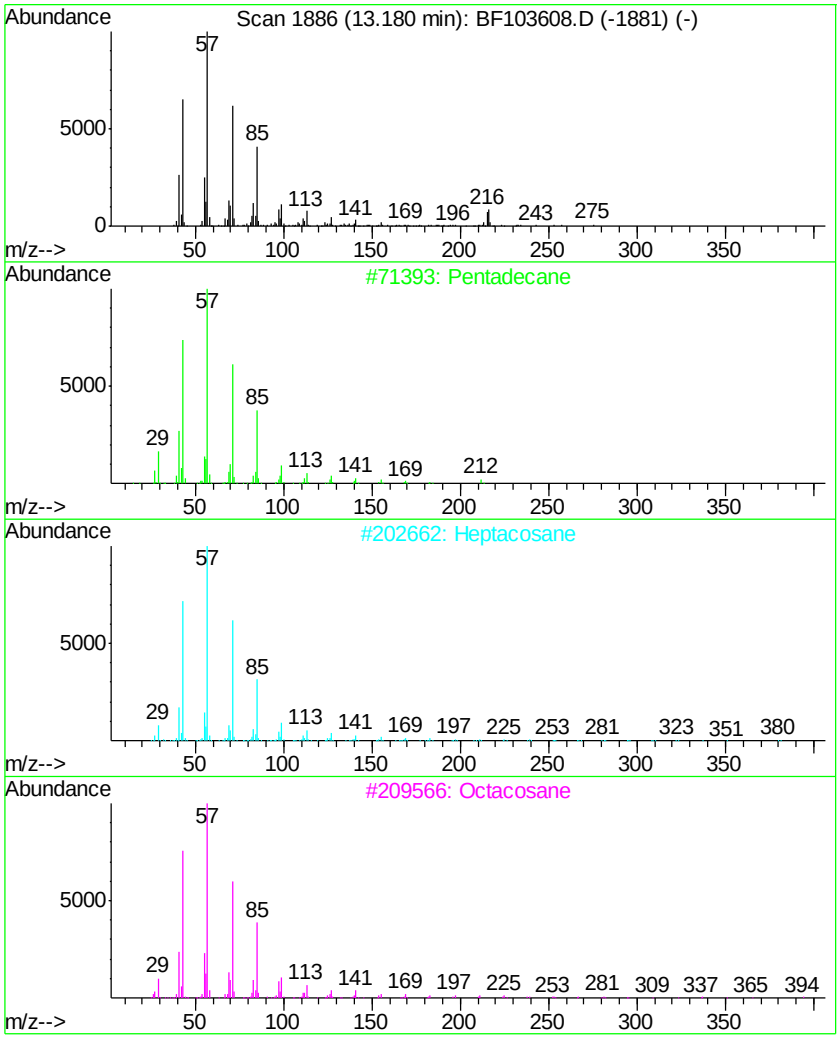
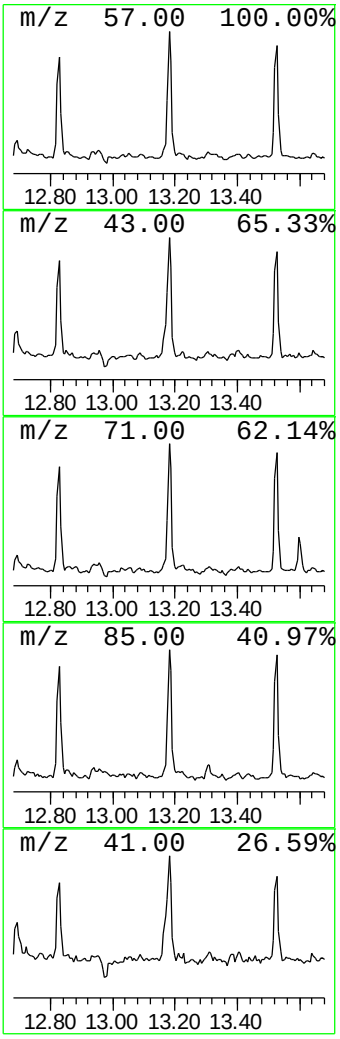
Peak Number 10 Pentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	9.00 ng	486176	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	94
2	Heptacosane	380	C27H56	000593-49-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Hexadecane	226	C16H34	000544-76-3	87





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Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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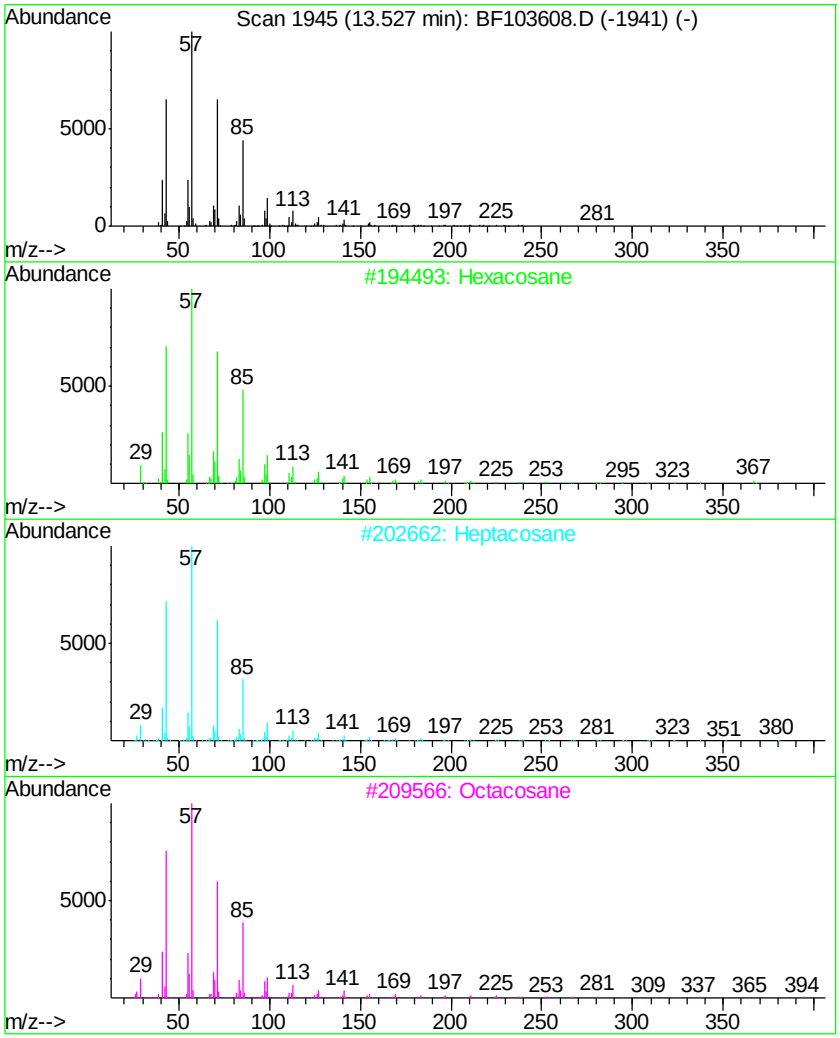
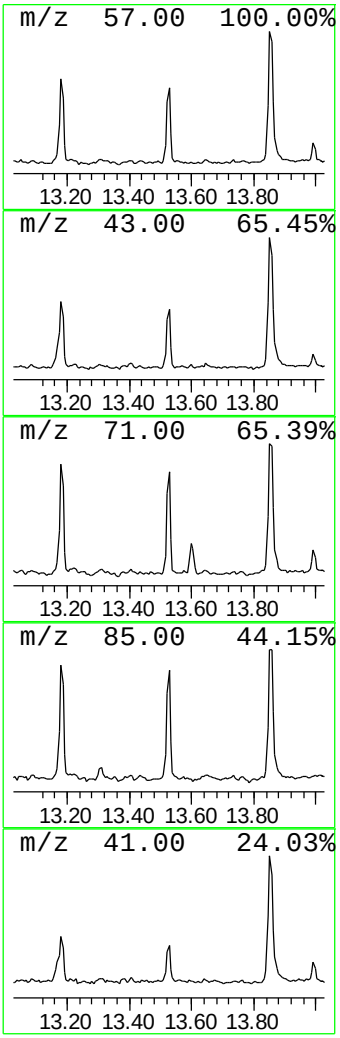
Peak Number 11 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	5.50 ng	297006	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90





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Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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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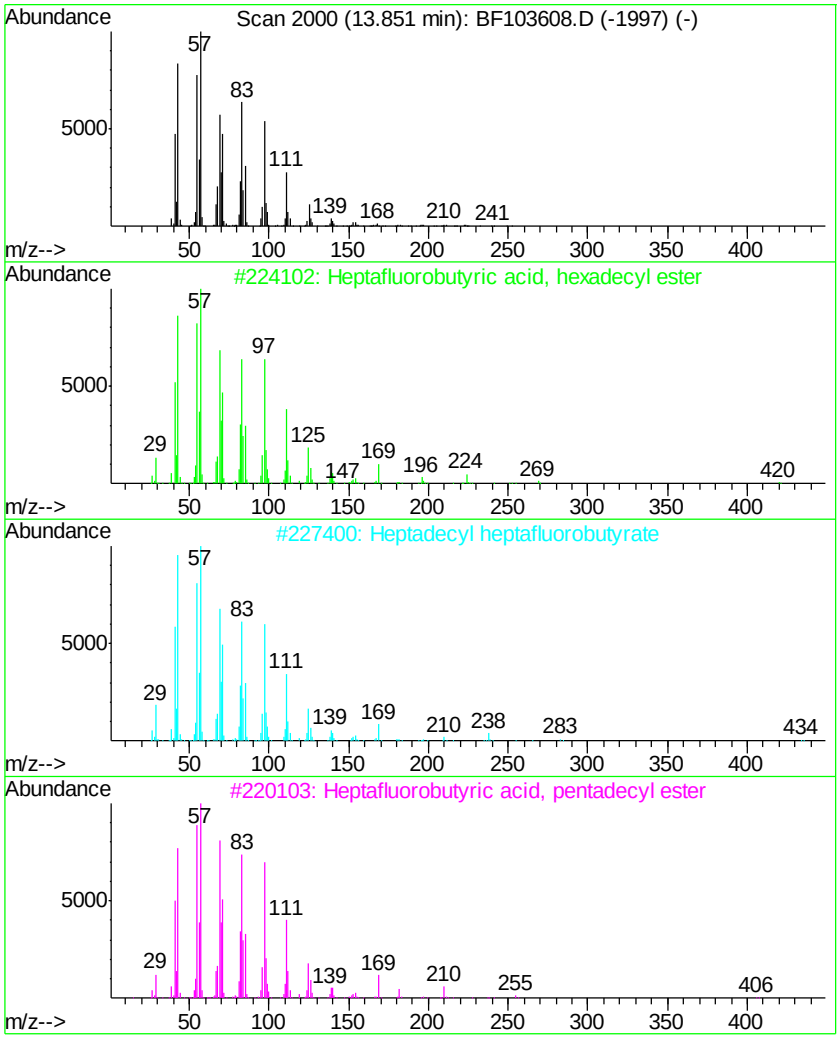
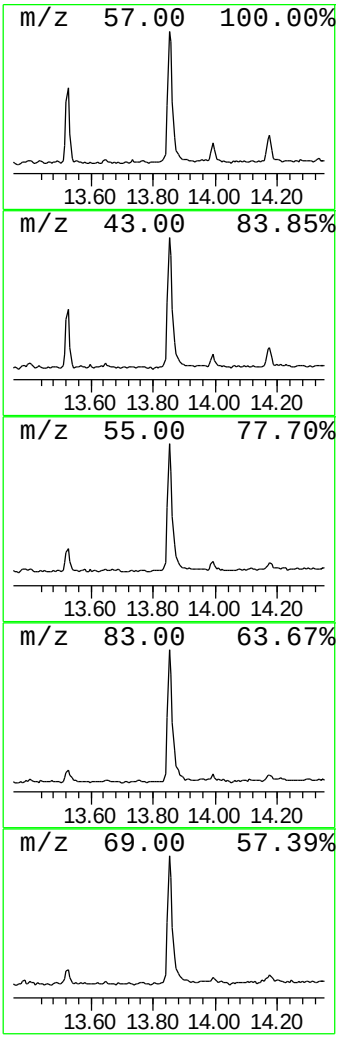
Peak Number 12 Heptafluorobutyric acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	22.43 ng	1212190	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91





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Operator : SJ/JU
Sample : J1890-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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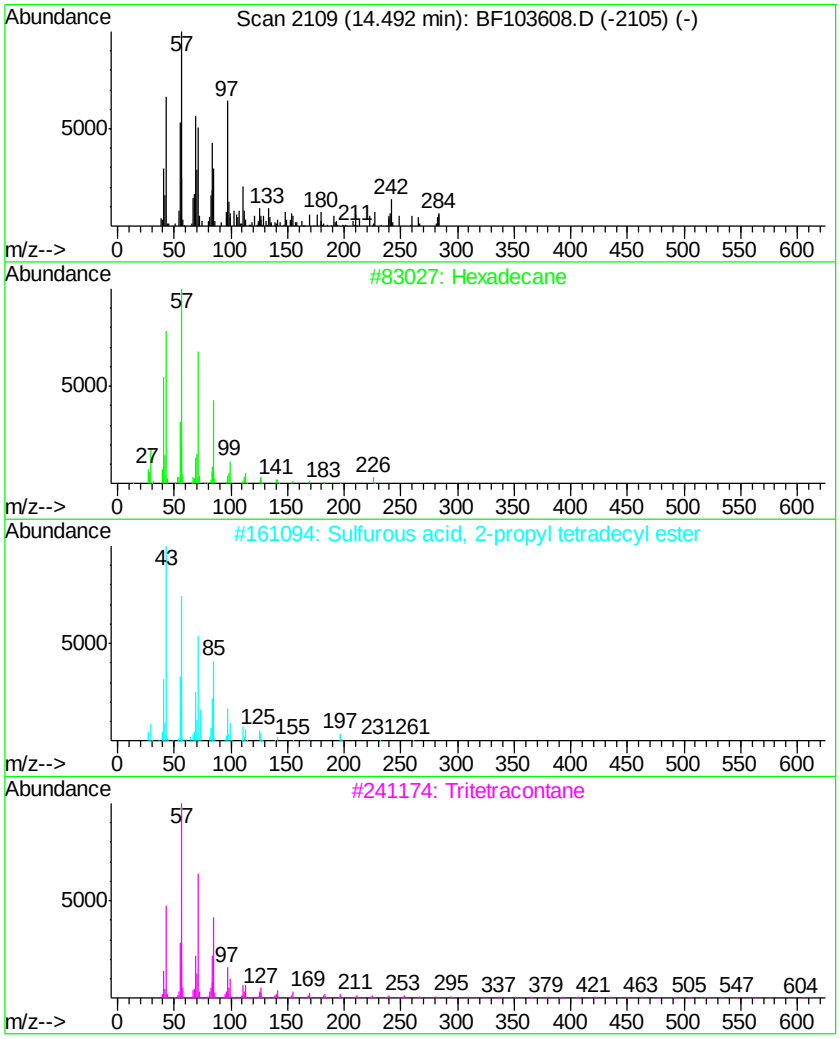
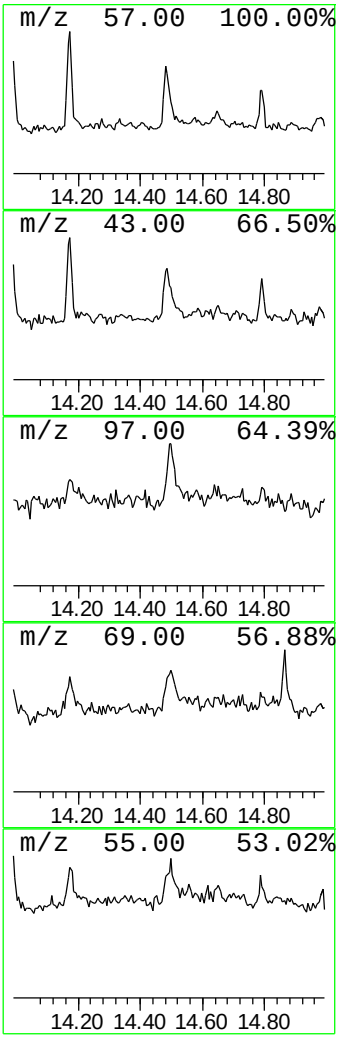
Peak Number 13 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.24 ng	120823	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	87
3	Tritetracontane	605	C43H88	007098-21-7	87
4	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	86
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	86





Tentatively Identified Compound (LSC) summary

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Data File : BF103608.D
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Operator : SJ/JU
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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
2-Pentanone, 4-hy...	5.10	2.2	ng	92052	1	6.86	831720	20.0
unknown6.63	6.63	88.5	ng	3679140	1	6.86	831720	20.0
Propanoic acid, 2...	9.07	3.4	ng	208034	3	9.90	1208360	20.0
2,4,7,9-Tetrameth...	9.32	2.5	ng	152069	3	9.90	1208360	20.0
Vanillin	9.39	3.9	ng	236427	3	9.90	1208360	20.0
Phthalic acid, 5-...	11.54	5.7	ng	339112	4	11.39	1183000	20.0
n-Tridecan-1-ol	11.59	2.2	ng	128881	4	11.39	1183000	20.0
Decane, 3-methyl-	12.45	2.2	ng	129370	4	11.39	1183000	20.0
Pentadecane	13.18	9.0	ng	486176	5	14.05	1080950	20.0
Hexacosane	13.53	5.5	ng	297006	5	14.05	1080950	20.0
Heptafluorobutyri...	13.85	22.4	ng	1212190	5	14.05	1080950	20.0
Hexadecane	14.49	2.2	ng	120823	5	14.05	1080950	20.0