LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082415\
Data File : BF081192.D
Acq On : 25 Aug 2015 3:43
Operator : UM/IZ
Sample : G3388-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5.5-6)BGS

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-BF081715.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	2.641	63	66	78	rBV2	5067	28948	1.20%	0.144%
2	3.898	173	176	181	rBV	15057	24894	1.03%	0.123%
3	4.653	238	242	254	rVB	794423	1441972	59.78%	7.151%
4	5.110	279	282	285	rBV	1735382	1974611	81.86%	9.793%
5	5.533	317	319	323	rVB	32074	29406	1.22%	0.146%
6	6.196	374	377	379	rBV	1938531	2412107	100.00%	11.962%
7	6.310	384	387	389	rBV	1892699	2156286	89.39%	10.694%
8	6.539	405	407	409	rBV	540256	436232	18.09%	2.163%
9	6.699	418	421	423	rBV	1558814	1553563	64.41%	7.705%
10	7.110	454	457	459	rBV	1349603	1305579	54.13%	6.475%
11	7.819	517	519	522	rBV	392877	515992	21.39%	2.559%
12	8.905	611	614	616	rBV	2215137	2102084	87.15%	10.425%
13	9.305	646	649	651	rBV	429667	379909	15.75%	1.884%
14	9.568	670	672	674	rVB	660035	588541	24.40%	2.919%
15	10.025	710	712	713	rVB	33311	27617	1.14%	0.137%
16	10.345	738	740	743	rBV2	890520	1251444	51.88%	6.206%
17	10.493	751	753	755	rBV	45510	51210	2.12%	0.254%
18	10.939	787	792	793	rBV	34492	35123	1.46%	0.174%
19	11.031	798	800	803	rVV2	501126	580976	24.09%	2.881%
20	11.305	822	824	827	rBV2	28095	72713	3.01%	0.361%
21	11.362	827	829	835	rVB	33471	45281	1.88%	0.225%
22	11.591	847	849	853	rBV	47667	62026	2.57%	0.308%
23	11.842	869	871	874	rVB	174641	150945	6.26%	0.749%
24	12.619	936	939	942	rBV	1765126	1872931	77.65%	9.288%
25	13.545	1018	1020	1027	rBV3	23258	98112	4.07%	0.487%
26	13.648	1027	1029	1031	rBV	643440	572963	23.75%	2.841%
27	14.974	1143	1145	1148	rBV	286432	392684	16.28%	1.947%

Sum of corrected areas: 20164149

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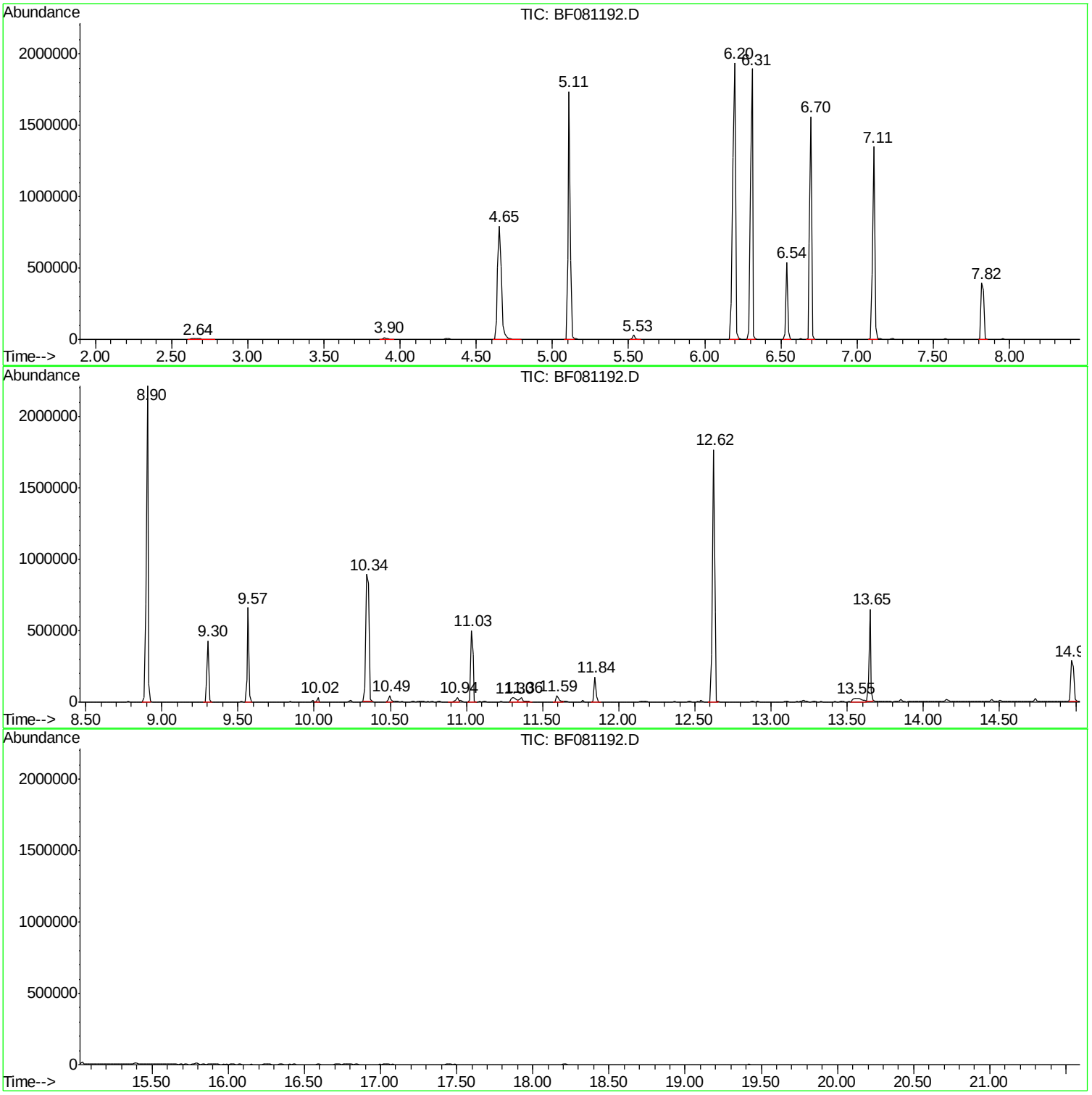
ClientSampleId :
SB-6(5.5-6)BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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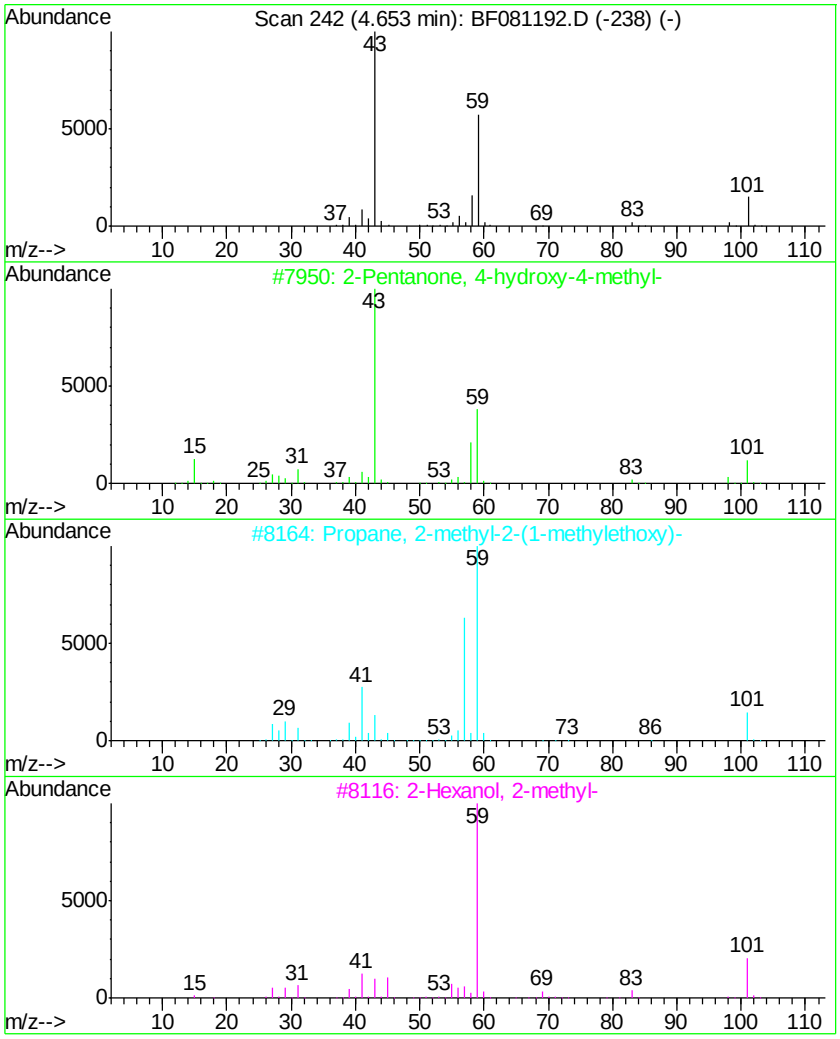
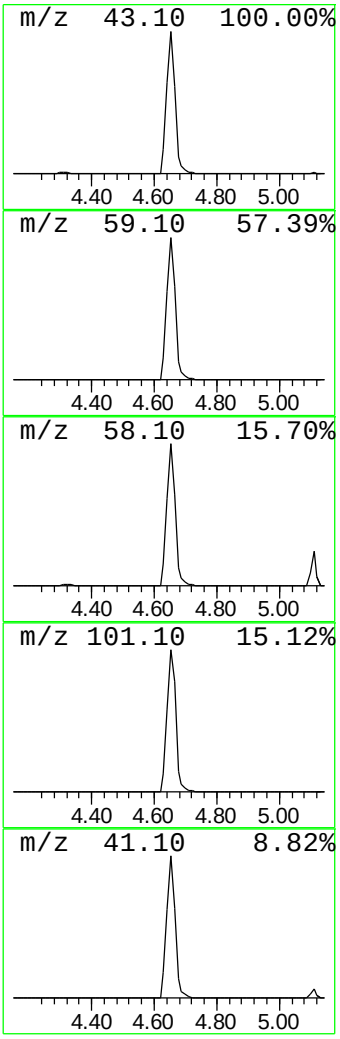
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	66.11 ng	1441970	1,4-Dichlorobenzene-d4	6.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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ClientSampleId : SB-6(5.5-6)BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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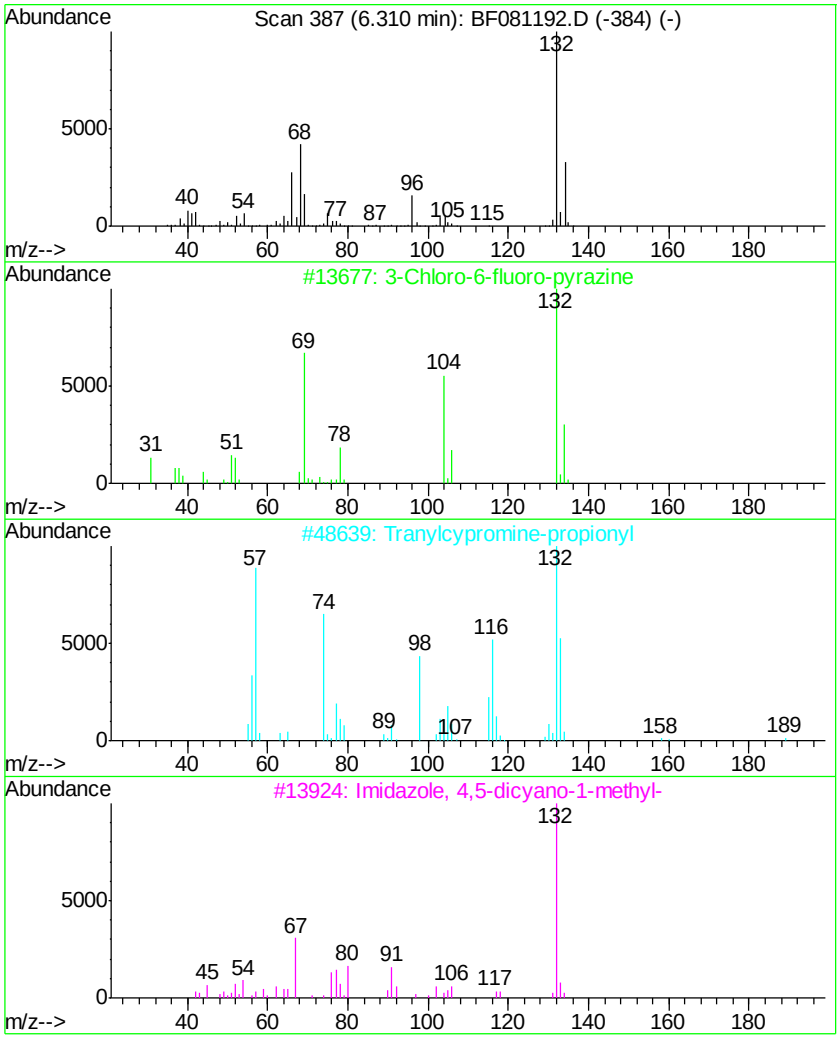
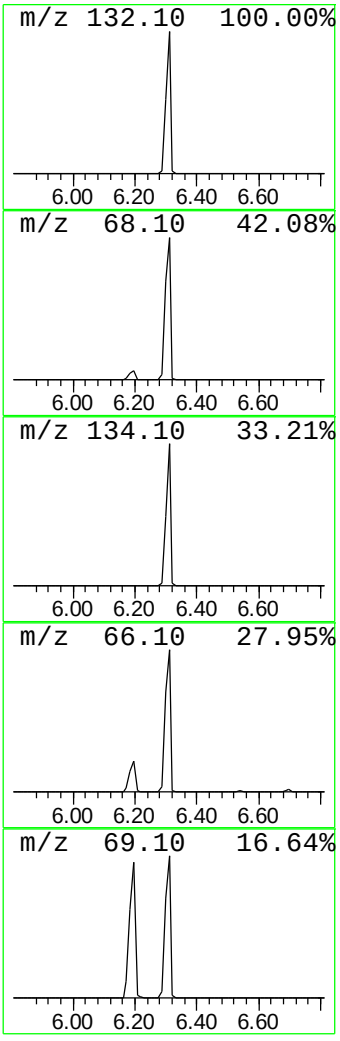
Peak Number 2 unknown6.31 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	98.86 ng	2156290	1,4-Dichlorobenzene-d4	6.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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ClientSampleId : SB-6(5.5-6)BGS

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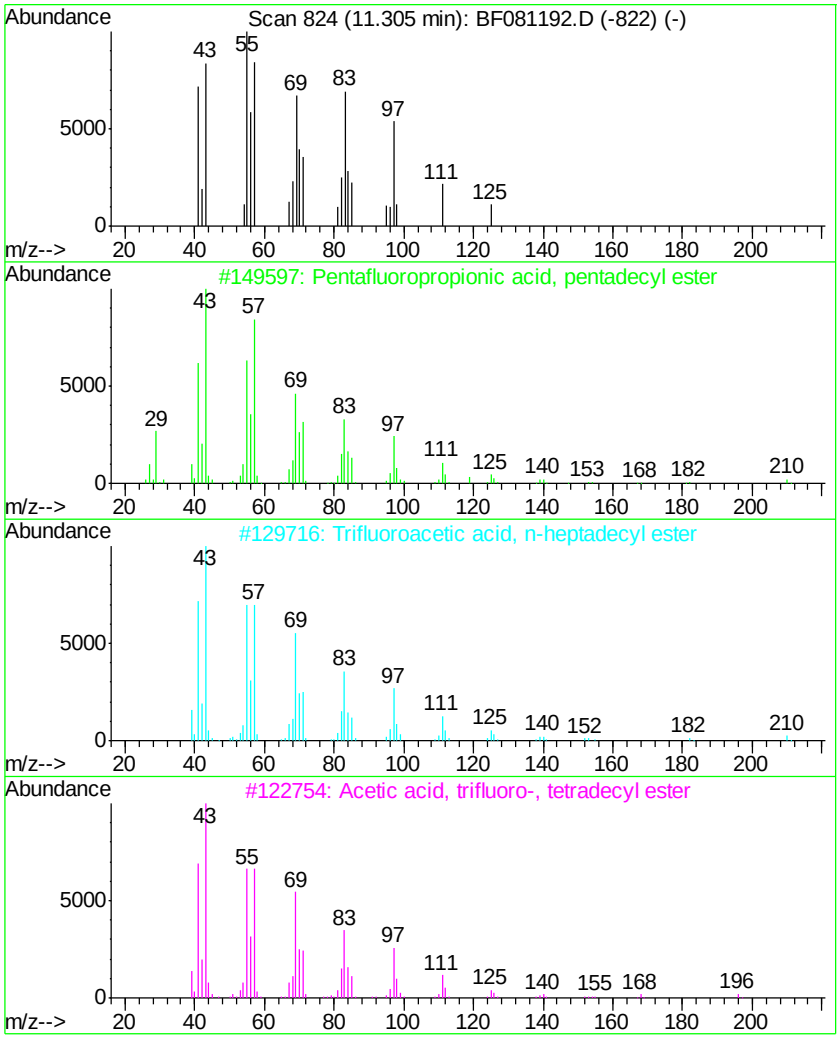
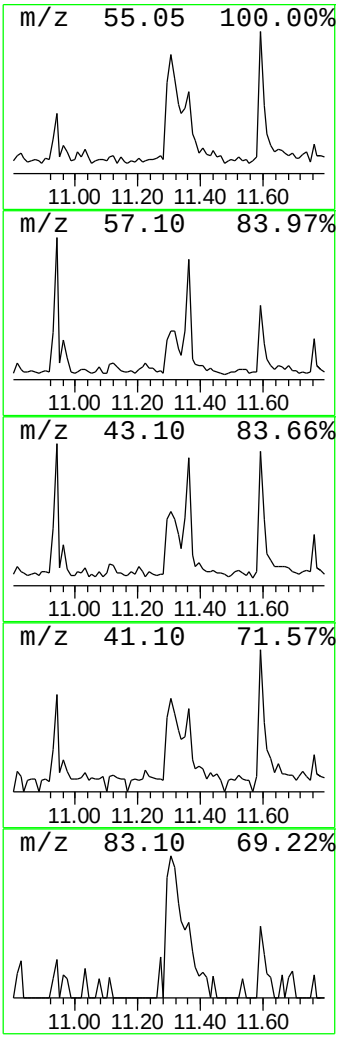
Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	2.50 ng	72713	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	86
2	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	83
3	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	83
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	80
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	72





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ClientSampleId : SB-6(5.5-6)BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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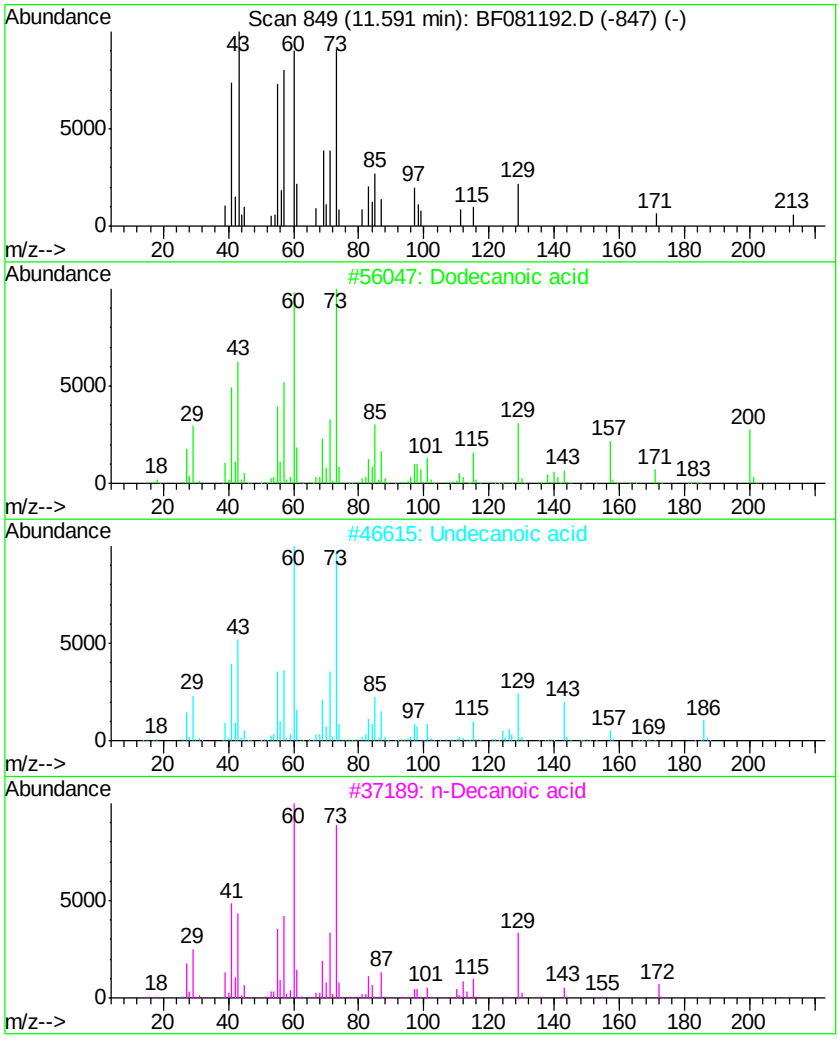
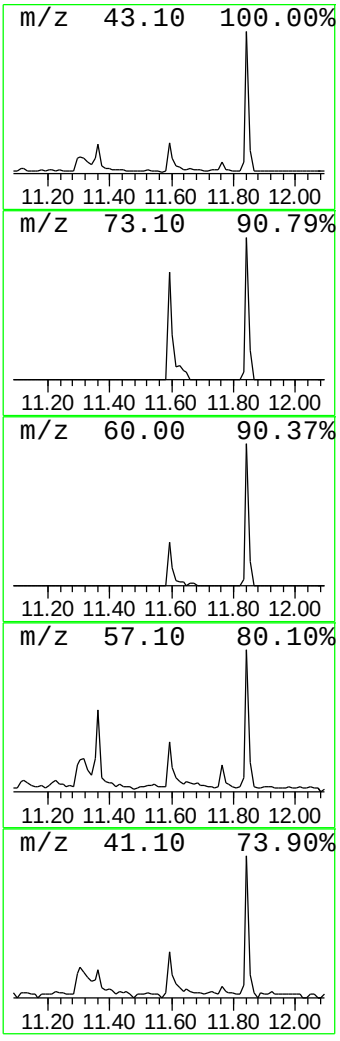
Peak Number 5 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.14 ng	62026	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	78
2	Undecanoic acid	186	C11H22O2	000112-37-8	78
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Undecane	156	C11H24	001120-21-4	14
5	Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	14





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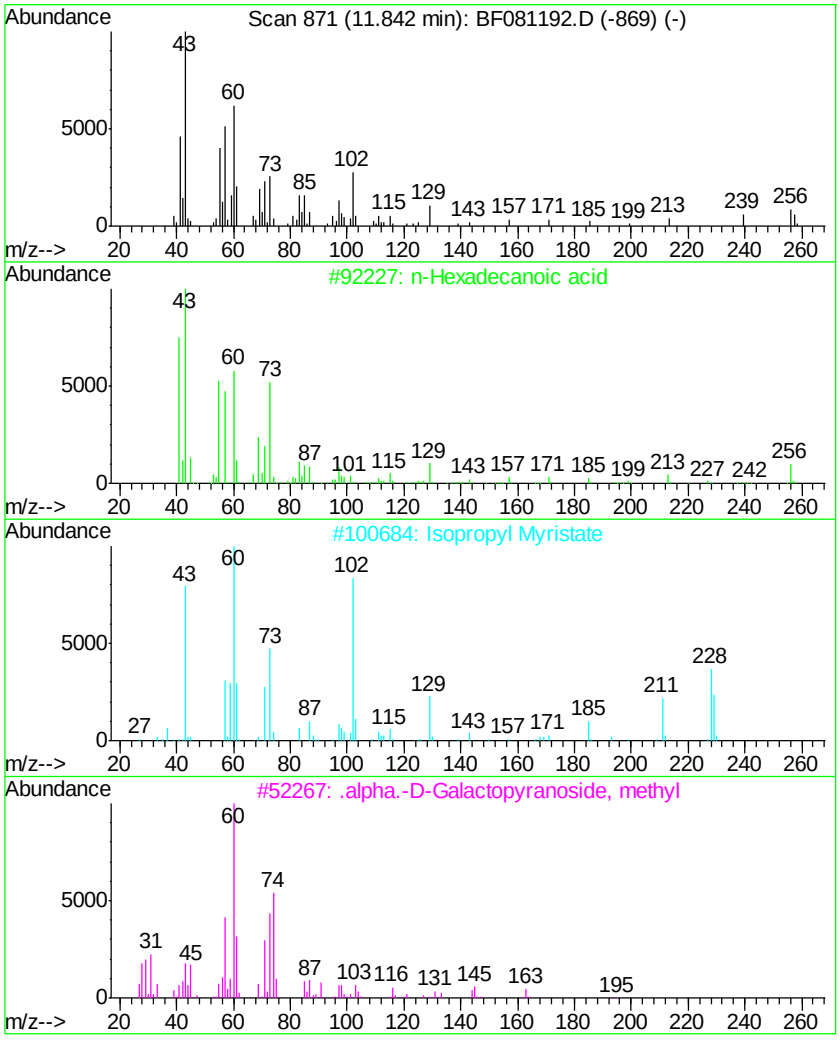
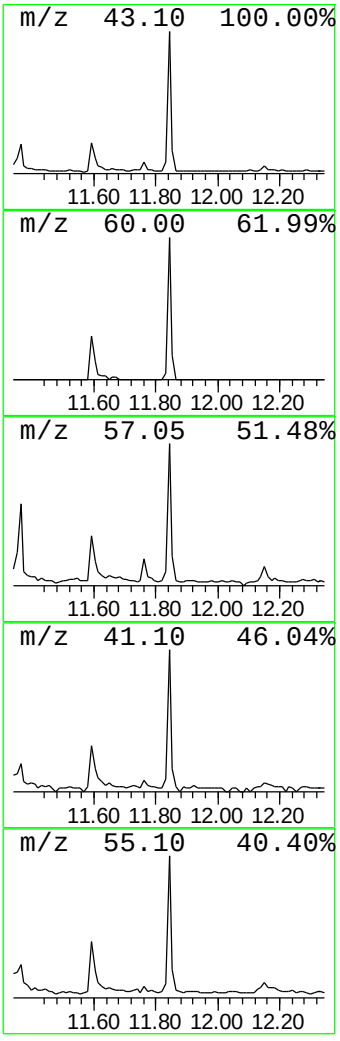
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	5.20 ng	150945	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Isopropyl Myristate	270	C17H34O2	000110-27-0	59
3	.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	50
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	50
5	Ethanole, 2-[(2-chloroethyl)thio...	182	C6H11ClO2S	006321-47-7	35





Library Search Compound Report

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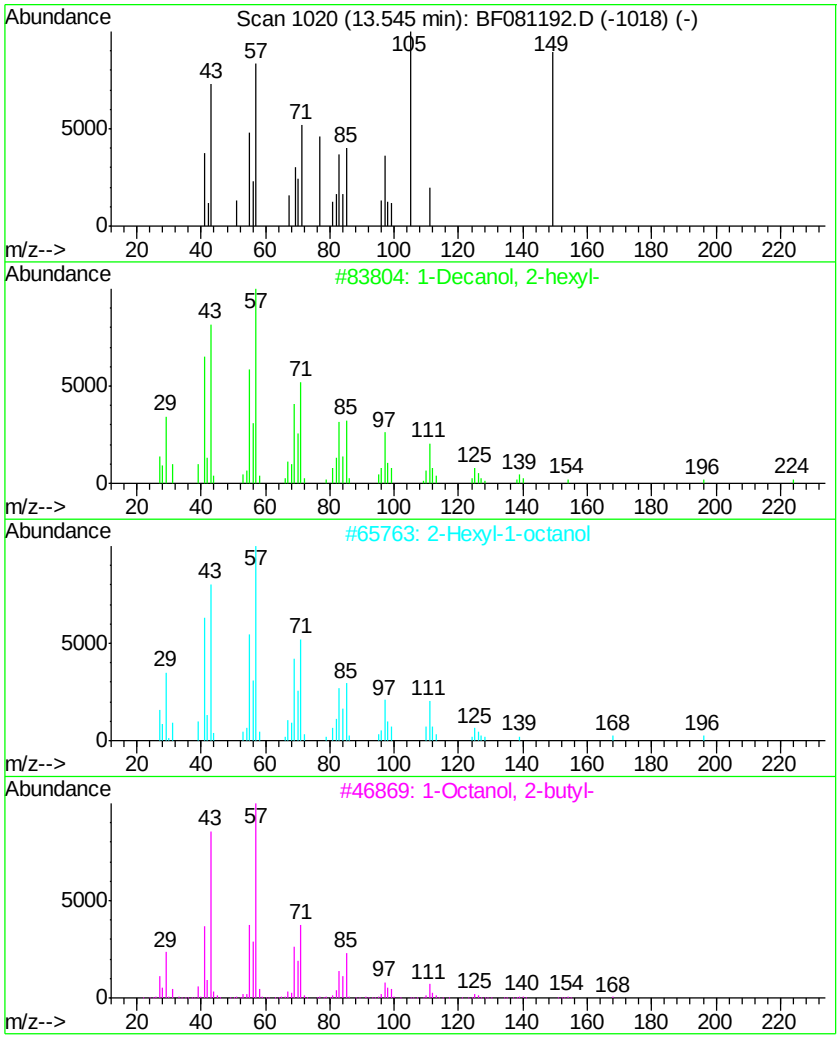
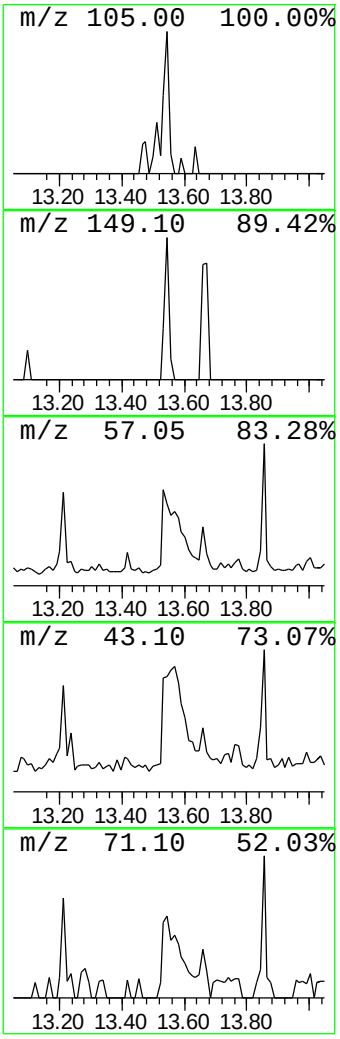
Peak Number 7 unknown13.55 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	3.42 ng	98112	Chrysene-d12	13.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
2	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	35
3	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	35
4	Nonadecane	268	C19H40	000629-92-5	22
5	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	22





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.65	66.1	ng	1441970	1	6.54	436232	20.0
unknown6.31	6.31	98.9	ng	2156290	1	6.54	436232	20.0
Pentafluoropropio...	11.30	2.5	ng	72713	4	11.03	580976	20.0
Dodecanoic acid	11.59	2.1	ng	62026	4	11.03	580976	20.0
n-Hexadecanoic acid	11.84	5.2	ng	150945	4	11.03	580976	20.0
unknown13.55	13.55	3.4	ng	98112	5	13.65	572963	20.0