LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104888.D
Acq On : 27 Apr 2018 18:24
Operator : JU/SJ
Sample : J2522-06
Misc :
ALS Vial : 10 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-BF040618.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	4.363	382	387	397	rBV	301141	355639	8.71%	1.787%
2	5.034	490	501	504	rBV	2042804	4083941	100.00%	20.526%
3	5.416	563	566	580	rBV	231508	251617	6.16%	1.265%
4	6.069	675	677	686	rVB	68201	65399	1.60%	0.329%
5	6.434	735	739	754	rBV	997500	1092843	26.76%	5.493%
6	6.569	758	762	766	rVB	504094	445761	10.91%	2.240%
7	6.798	797	801	804	rBV	653902	599730	14.69%	3.014%
8	6.951	823	827	830	rBV	1693878	1429831	35.01%	7.186%
9	7.363	891	897	905	rBV	1205986	1098123	26.89%	5.519%
10	8.081	1015	1019	1037	rVB	891561	826207	20.23%	4.153%
11	9.157	1198	1202	1205	rBV	2330423	2047844	50.14%	10.293%
12	9.551	1264	1269	1277	rBV	103374	117061	2.87%	0.588%
13	9.839	1314	1318	1331	rVB	897855	890553	21.81%	4.476%
14	10.257	1386	1389	1392	rBV	53829	41573	1.02%	0.209%
15	10.733	1467	1470	1479	rVB	58005	60436	1.48%	0.304%
16	11.327	1567	1571	1586	rVB	881024	818473	20.04%	4.114%
17	12.916	1836	1841	1844	rBV	1773333	1613575	39.51%	8.110%
18	13.098	1869	1872	1881	rVB2	48301	78709	1.93%	0.396%
19	13.198	1887	1889	1893	rVB	53071	50146	1.23%	0.252%
20	13.310	1904	1908	1912	rBV	46833	49557	1.21%	0.249%
21	13.392	1917	1922	1925	rVV	2454902	2242631	54.91%	11.272%
22	13.663	1965	1968	1970	rBV	59723	63318	1.55%	0.318%
23	13.727	1977	1979	1982	rVB	62220	53586	1.31%	0.269%
24	13.768	1982	1986	1988	rBV2	42344	50567	1.24%	0.254%
25	13.798	1988	1991	1994	rBV	109359	115662	2.83%	0.581%
26	13.839	1994	1998	2001	rVB	127581	142830	3.50%	0.718%
27	13.974	2017	2021	2025	rVV	622415	580564	14.22%	2.918%
28	15.439	2265	2270	2277	rBV	467734	630095	15.43%	3.167%

Sum of corrected areas: 19896271

LSC Report - Integrated Chromatogram

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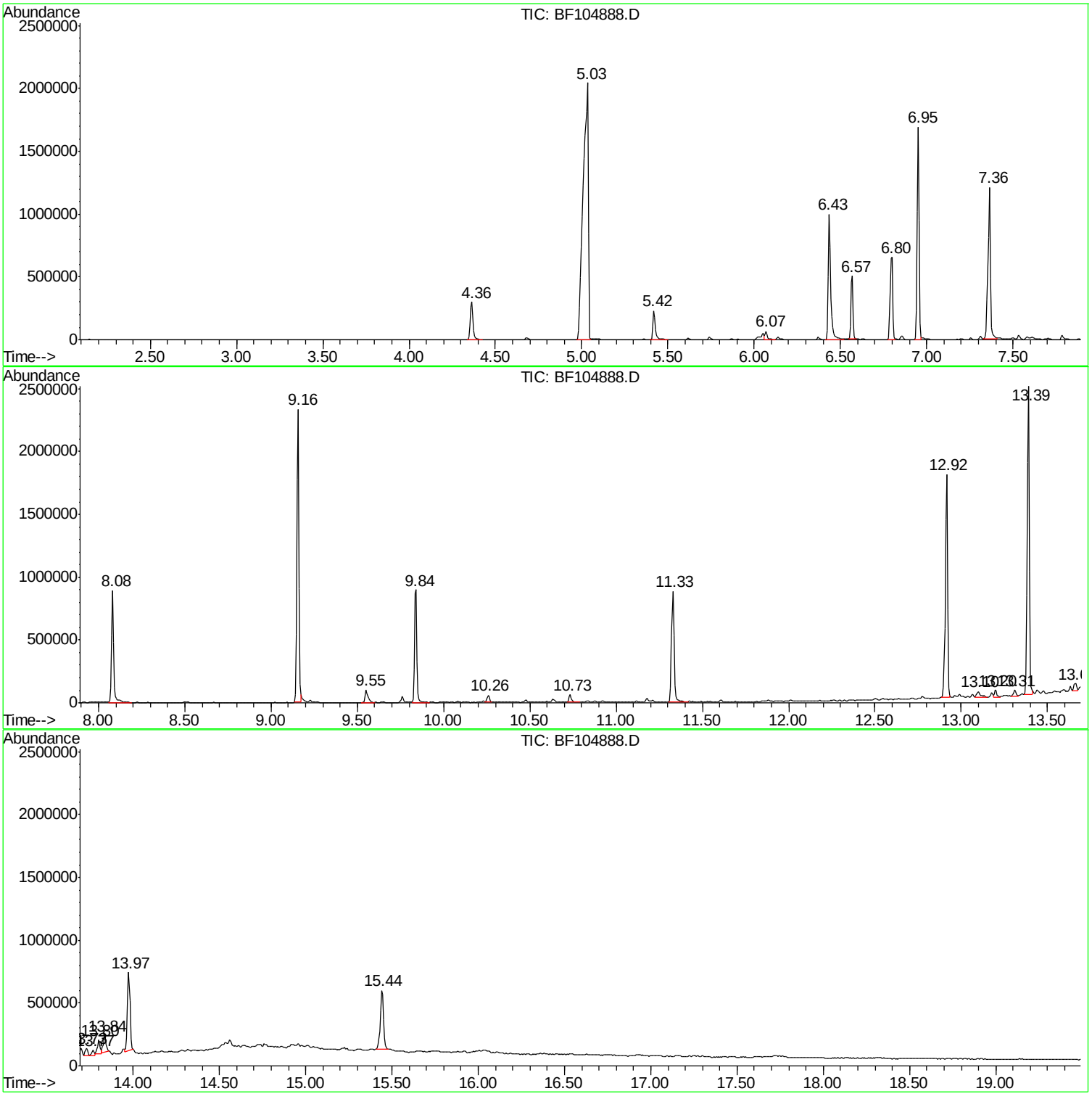
Operator : JU/SJ
Sample : J2522-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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\BF042718\
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Operator : JU/SJ
Sample : J2522-06
Misc :
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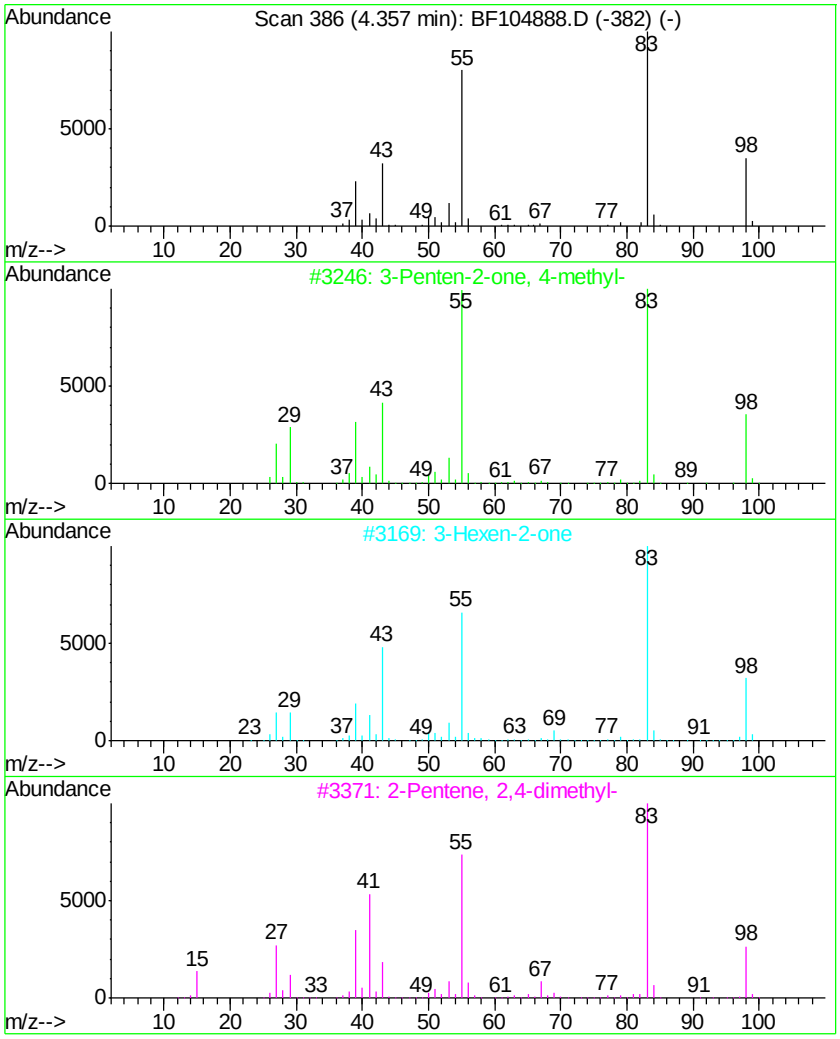
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

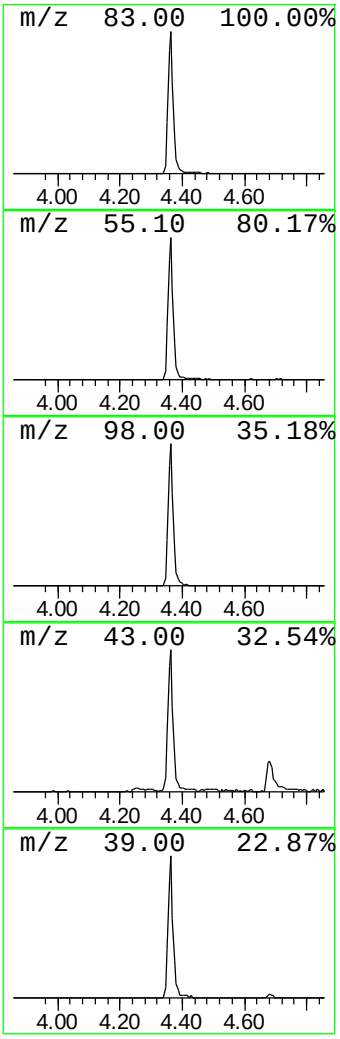
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	11.86 ng	355639	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Data File : BF104888.D
Acq On : 27 Apr 2018 18:24
Operator : JU/SJ
Sample : J2522-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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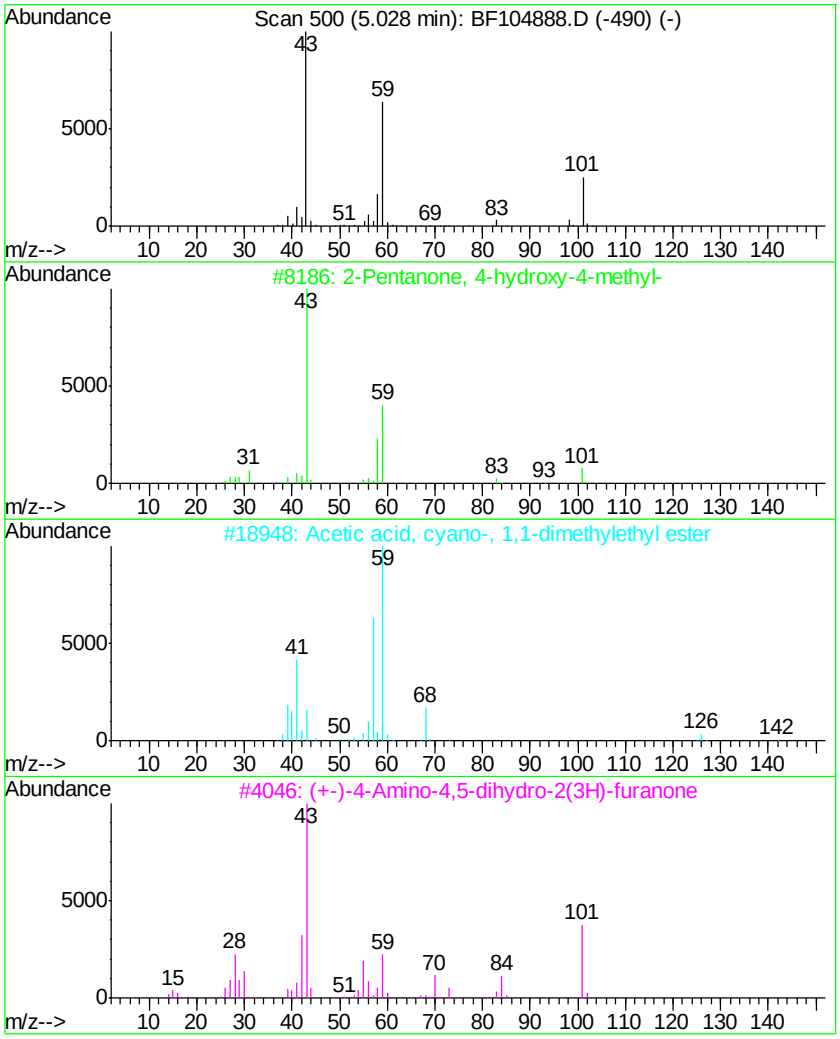
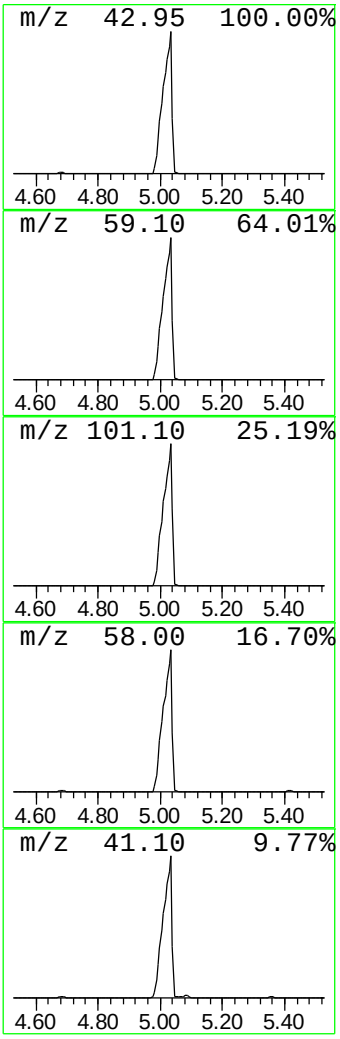
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	136.19 ng	4083940	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104888.D
Acq On : 27 Apr 2018 18:24
Operator : JU/SJ
Sample : J2522-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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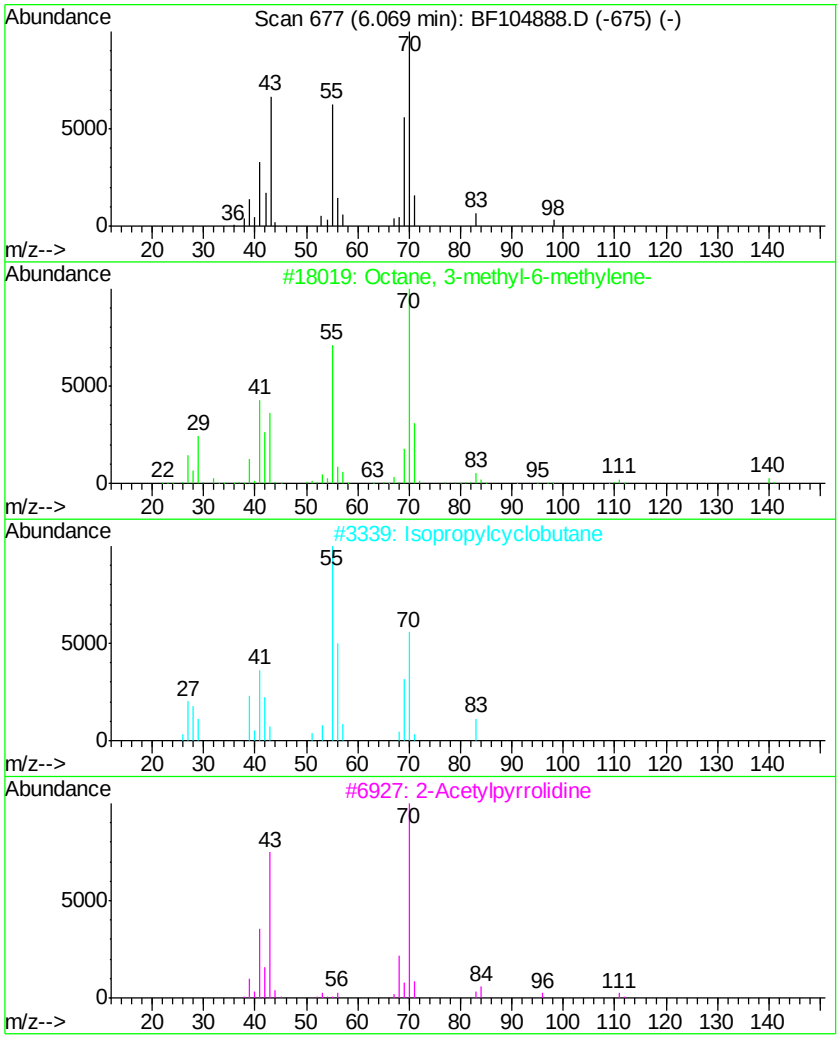
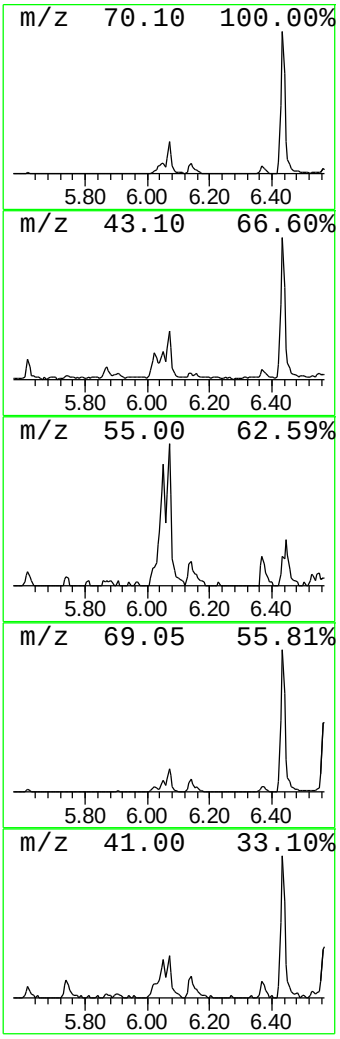
Peak Number 3 Octane, 3-methyl-6-methylene- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.07	2.18 ng	65399	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-6-methylene-	140	C10H20	074630-07-2	72
2	Isopropylcyclobutane	98	C7H14	000872-56-0	59
3	2-Acetylpyrrolidine	113	C6H11NO	060026-20-2	45
4	Undecane, 3-methylene-	168	C12H24	071138-64-2	43
5	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104888.D
Acq On : 27 Apr 2018 18:24
Operator : JU/SJ
Sample : J2522-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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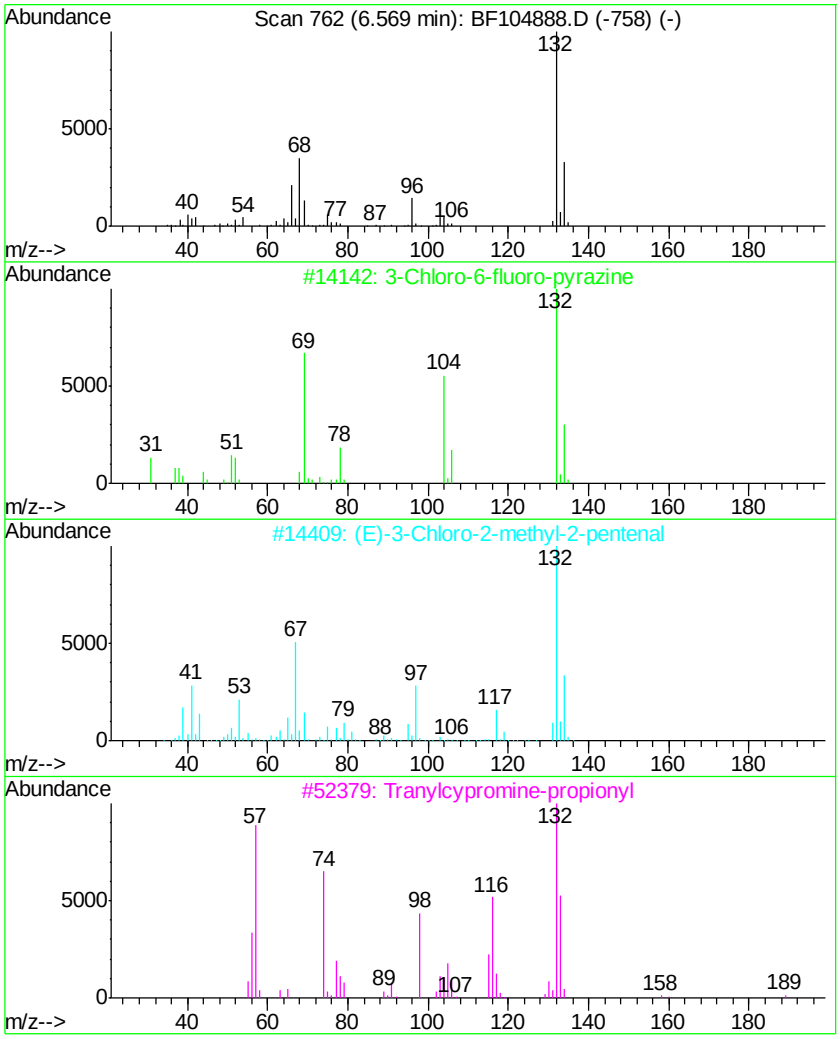
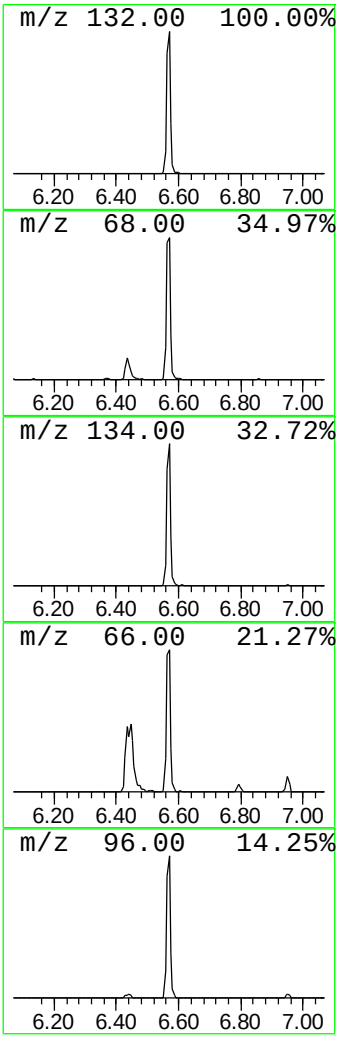
Peak Number 4 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	14.87 ng	445761	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104888.D
Acq On : 27 Apr 2018 18:24
Operator : JU/SJ
Sample : J2522-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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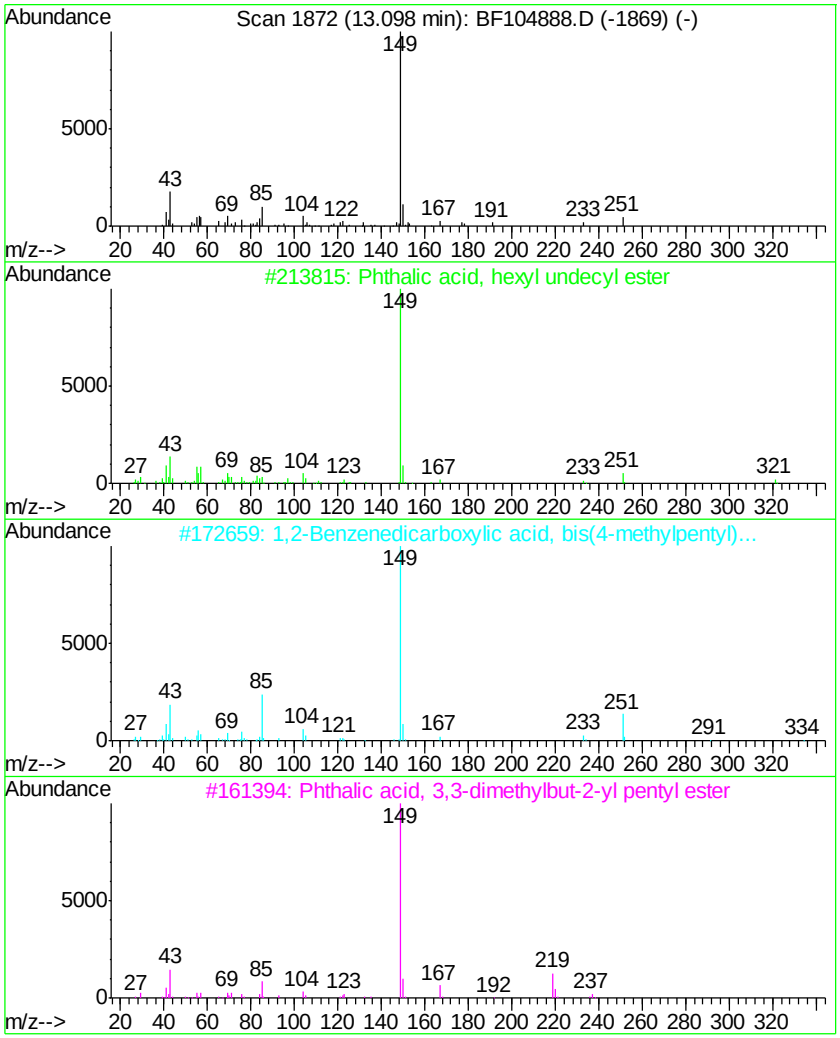
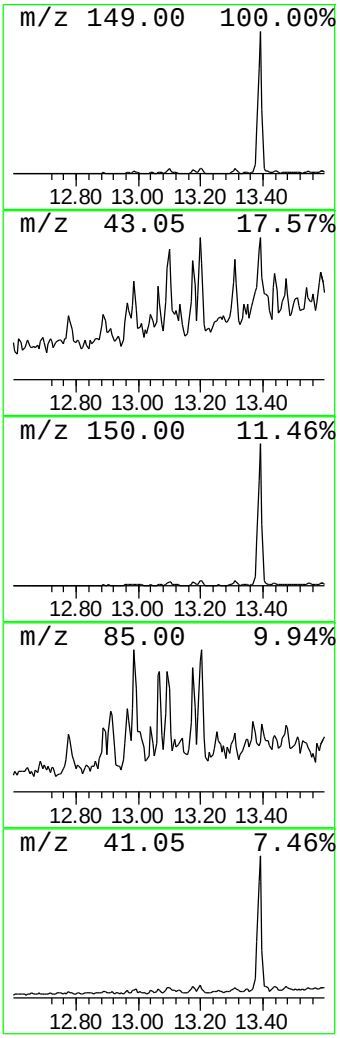
Peak Number 6 Phthalic acid, hexyl undecy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	2.71 ng	78709	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, hexyl undecyl ester	404	C25H40O4	1000308-91-6	78
2	1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	78
3	Phthalic acid, 3,3-dimethylbut-2...	320	C19H28O4	1000357-00-3	78
4	Phthalic acid, 3,3-dimethylbut-2...	348	C21H32O4	1000357-00-6	78
5	1,2-Benzenedicarboxylic acid, de...	390	C24H38O4	025724-58-7	72





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Operator : JU/SJ
Sample : J2522-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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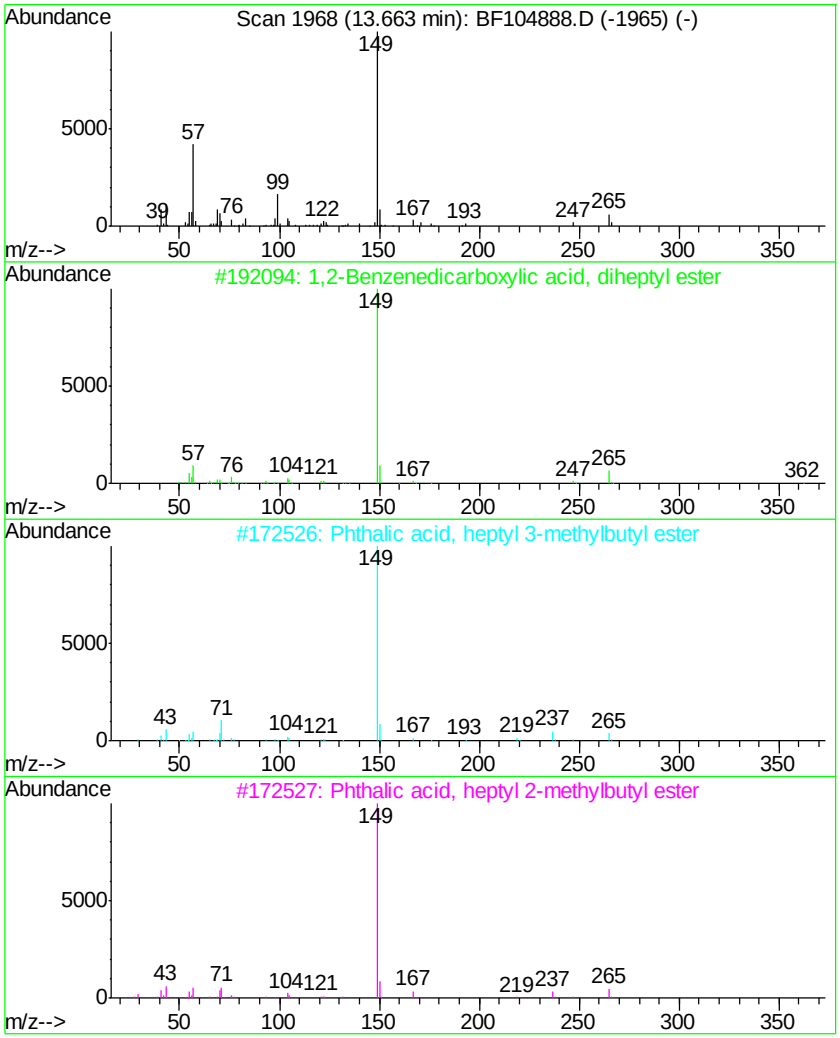
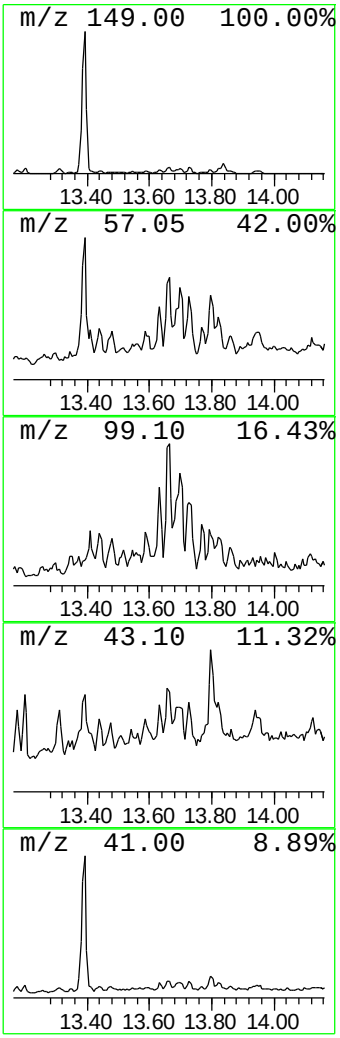
Peak Number 7 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	2.18 ng	63318	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	362	C22H34O4	003648-21-3	72
2	Phthalic acid, heptyl 3-methylbu...	334	C20H30O4	1000356-80-8	64
3	Phthalic acid, heptyl 2-methylbu...	334	C20H30O4	1000322-81-5	64
4	Phthalic acid, heptyl 4-octyl ester	376	C23H36O4	1000314-84-1	64
5	Phthalic acid, hexyl 2-methylpen...	334	C20H30O4	1000356-91-1	59





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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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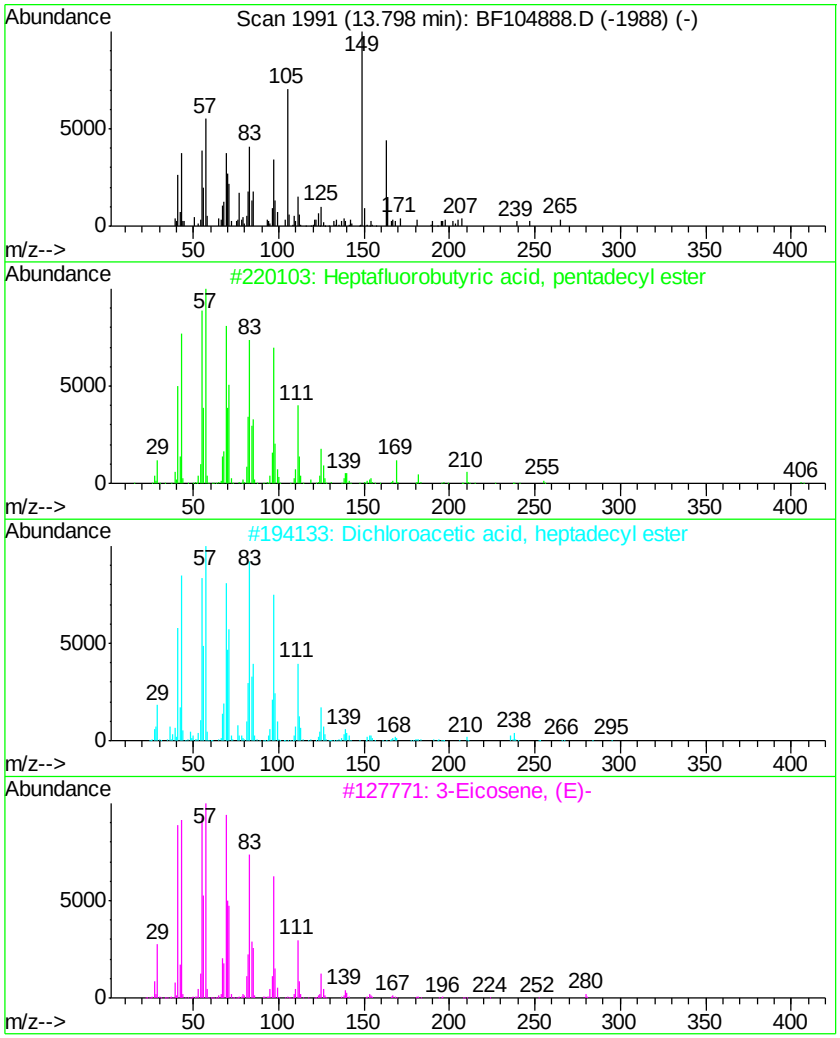
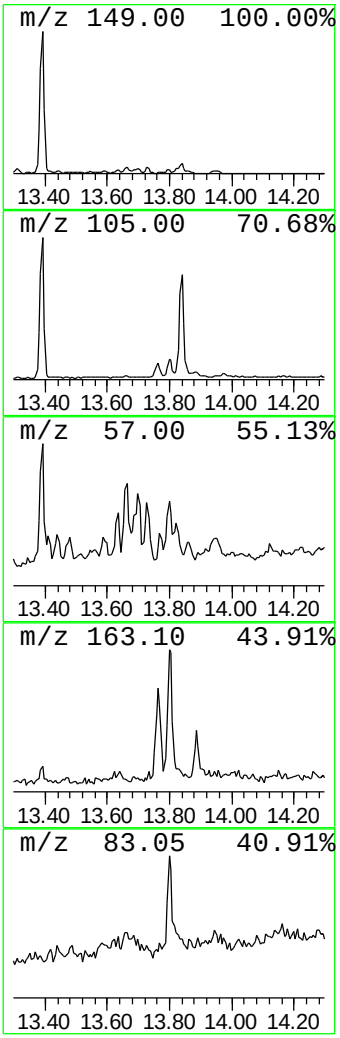
Peak Number 8 unknown13.80 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.98 ng	115662	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	46
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	46
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	42
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	41
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	41





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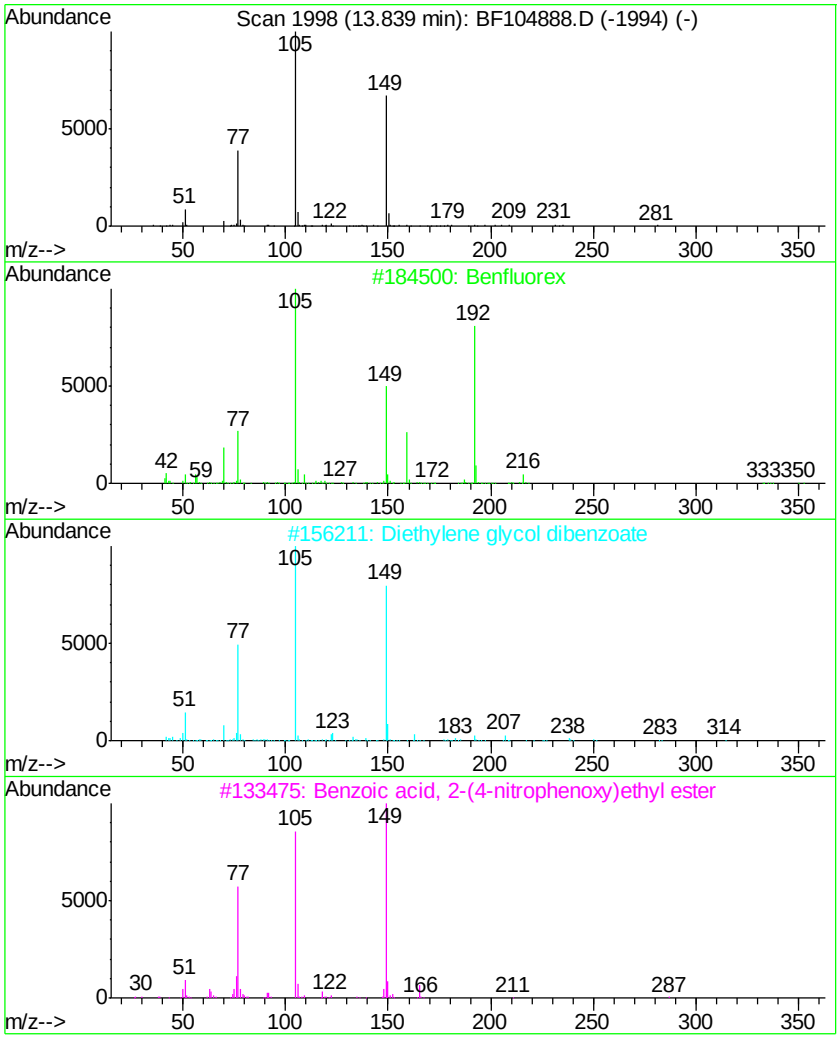
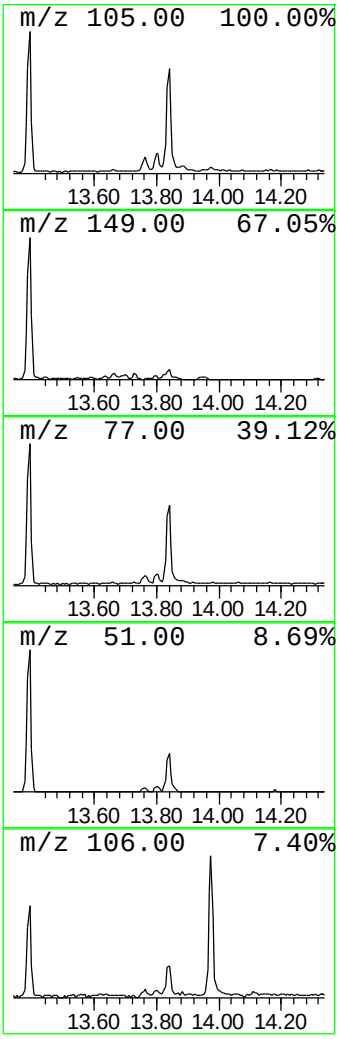
Peak Number 9 Benfluorex Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	4.92 ng	142830	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benfluorex	351	C19H20F3NO2	023602-78-0	78
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	50
4	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
5	N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	47





Tentatively Identified Compound (LSC) summary

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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
3-Penten-2-one, 4...	4.36	11.9	ng	355639	1	6.80	599730	20.0
2-Pentanone, 4-hy...	5.03	136.2	ng	4083940	1	6.80	599730	20.0
Octane, 3-methyl-...	6.07	2.2	ng	65399	1	6.80	599730	20.0
unknown6.57	6.57	14.9	ng	445761	1	6.80	599730	20.0
Phthalic acid, he...	13.10	2.7	ng	78709	5	13.97	580564	20.0
1,2-Benzenedicarb...	13.66	2.2	ng	63318	5	13.97	580564	20.0
unknown13.80	13.80	4.0	ng	115662	5	13.97	580564	20.0
Benfluorex	13.84	4.9	ng	142830	5	13.97	580564	20.0