LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

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-BF052316.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	2.181	50	52	58	rVB	56006	95329	2.72%	0.371%
2	4.741	274	276	292	rBV2	20827	111590	3.18%	0.435%
3	5.073	302	305	318	rBV2	35073	102035	2.91%	0.398%
4	5.404	331	334	352	rBV	353988	1184508	33.77%	4.615%
5	5.633	352	354	358	rVV	39480	88429	2.52%	0.345%
6	5.736	361	363	373	rVB5	10103	46139	1.32%	0.180%
7	6.993	471	473	477	rBV2	25897	47586	1.36%	0.185%
8	7.062	477	479	483	rVV	295296	568145	16.20%	2.213%
9	7.130	483	485	504	rVB	1471636	2820680	80.42%	10.989%
10	7.473	513	515	522	rBV	470860	696450	19.86%	2.713%
11	7.565	522	523	527	rVB	25294	40534	1.16%	0.158%
12	7.702	532	535	542	rVV	1802036	2506555	71.46%	9.765%
13	7.805	542	544	550	rVV	50229	88669	2.53%	0.345%
14	7.942	550	556	559	rVV3	28537	98771	2.82%	0.385%
15	8.010	559	562	572	rVB6	28160	100305	2.86%	0.391%
16	8.387	593	595	603	rBV	1270497	1871809	53.37%	7.292%
17	8.548	605	609	610	rVV2	113948	317311	9.05%	1.236%
18	8.605	610	614	621	rVB2	193335	564666	16.10%	2.200%
19	8.868	633	637	644	rVB	141186	255971	7.30%	0.997%
20	9.016	648	650	654	rVV3	19955	38521	1.10%	0.150%
21	9.108	654	658	664	rVB3	26187	61760	1.76%	0.241%
22	9.416	683	685	691	rVB2	42097	82952	2.37%	0.323%
23	9.508	691	693	704	rBV	542730	939897	26.80%	3.662%
24	9.942	723	731	733	rBV7	12837	40800	1.16%	0.159%
25	10.571	783	786	790	rBV3	15289	44778	1.28%	0.174%
26	10.708	796	798	804	rVB3	31513	57185	1.63%	0.223%
27	10.811	804	807	810	rBV2	24621	41568	1.19%	0.162%
28	10.879	810	813	820	rVV2	43013	125761	3.59%	0.490%
29	11.005	820	824	828	rVB4	29448	76934	2.19%	0.300%
30	11.108	828	833	835	rBV5	15423	44238	1.26%	0.172%
31	11.165	835	838	845	rVV2	62835	170733	4.87%	0.665%
32	11.279	845	848	857	rVB	2809247	3507479	100.00%	13.665%
33	11.748	886	889	892	rBV2	26214	60769	1.73%	0.237%
34	11.919	902	904	908	rBV3	13096	35895	1.02%	0.140%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : GMW-03

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.988	908	910	918	rVV	71352	134357	3.83%	0.523%
36	12.228	929	931	934	rBV3	21431	41803	1.19%	0.163%
37	12.331	938	940	949	rVV	698543	991706	28.27%	3.864%
38	12.731	970	975	980	rVV5	16205	61701	1.76%	0.240%
39	12.857	983	986	990	rVB4	15988	41615	1.19%	0.162%
40	13.097	1003	1007	1011	rBV2	43585	91294	2.60%	0.356%
41	13.154	1011	1012	1014	rVV	40823	51280	1.46%	0.200%
42	13.257	1018	1021	1025	rBV	61516	83055	2.37%	0.324%
43	13.622	1051	1053	1069	rBV	1086497	2060890	58.76%	8.029%
44	13.931	1078	1080	1084	rBV	47414	66482	1.90%	0.259%
45	14.742	1149	1151	1166	rVB	526263	869321	24.78%	3.387%
46	15.725	1235	1237	1244	rBV	30896	68506	1.95%	0.267%
47	17.086	1354	1356	1365	rBV	2245234	2732691	77.91%	10.646%
48	17.920	1425	1429	1432	rBV	42522	58137	1.66%	0.226%
49	18.343	1463	1466	1471	rBV3	18529	44395	1.27%	0.173%
50	18.468	1474	1477	1492	rBV	271229	696212	19.85%	2.712%
51	20.149	1622	1624	1635	rBV	221194	562917	16.05%	2.193%
52	21.120	1707	1709	1718	rVB3	21163	77020	2.20%	0.300%

Sum of corrected areas: 25668134

LSC Report - Integrated Chromatogram

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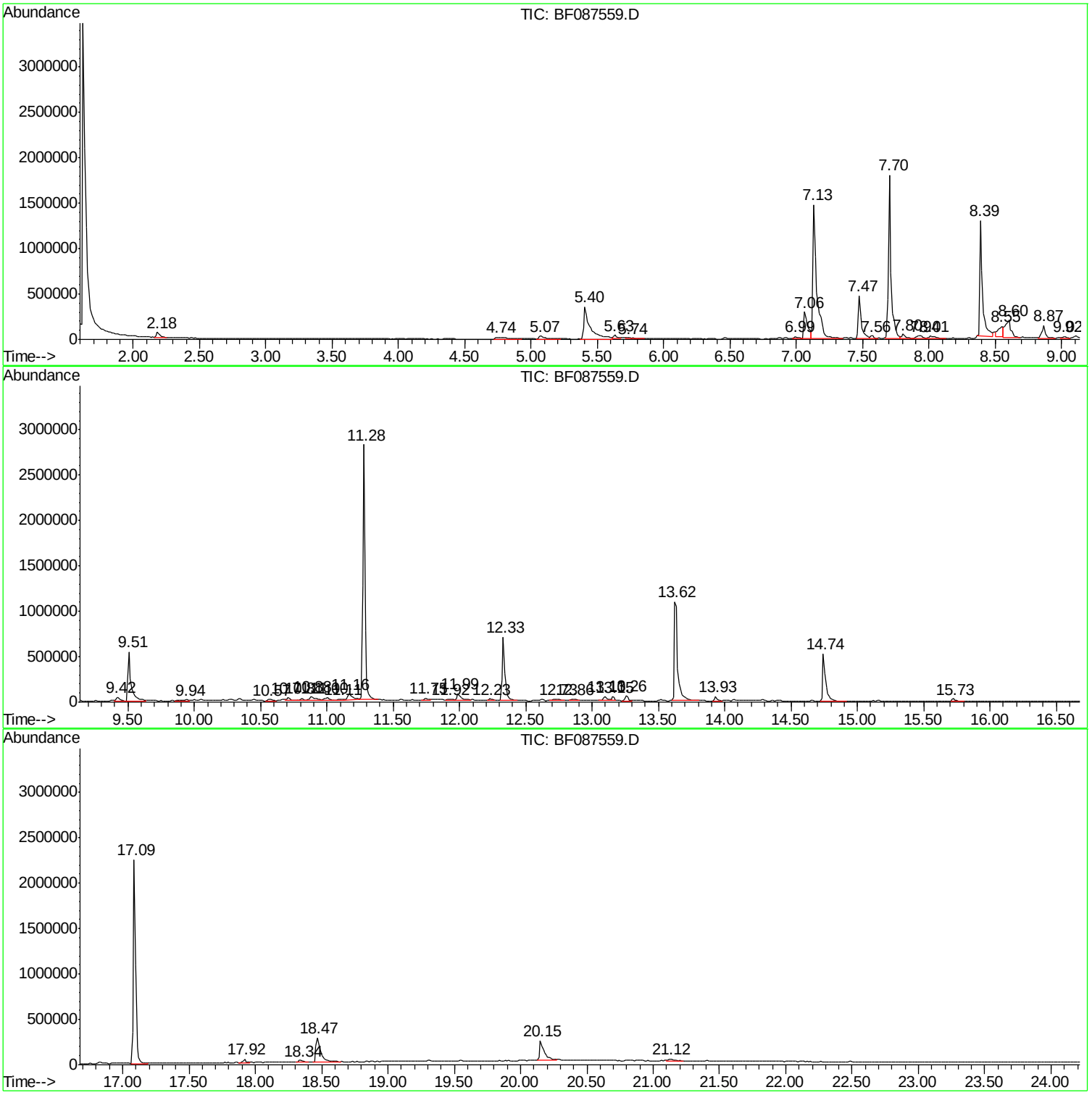
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

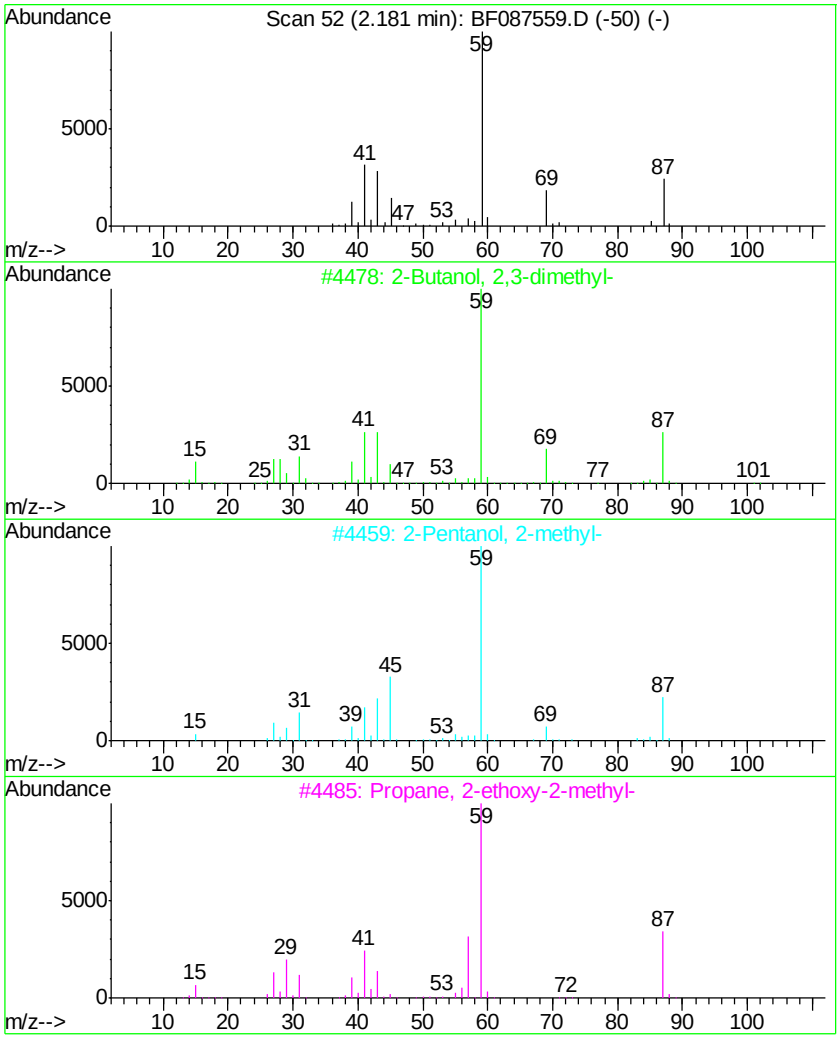
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

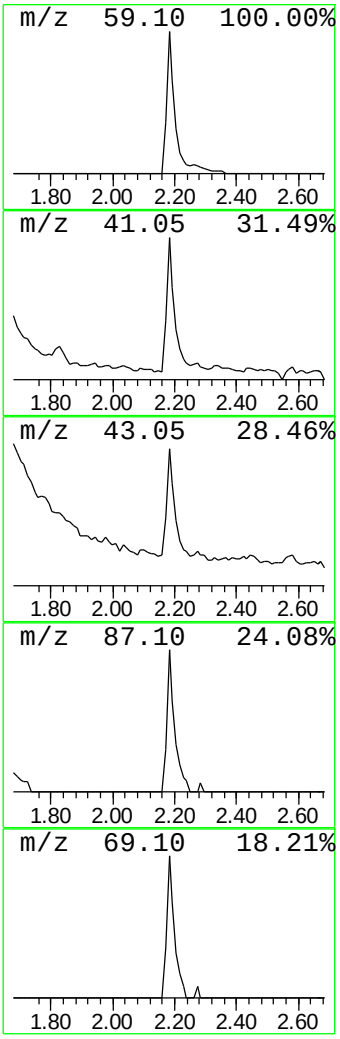
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	2.74 ng	95329	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
4	3-Heptanol	116	C7H16O	000589-82-2	39
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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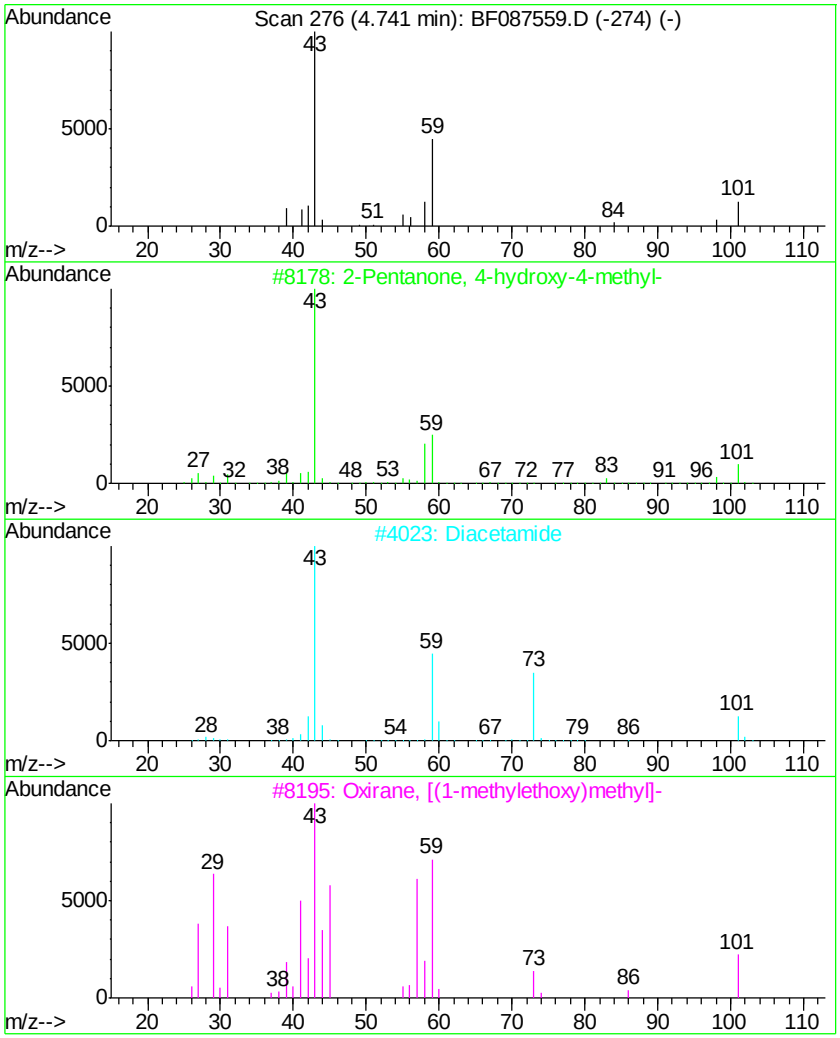
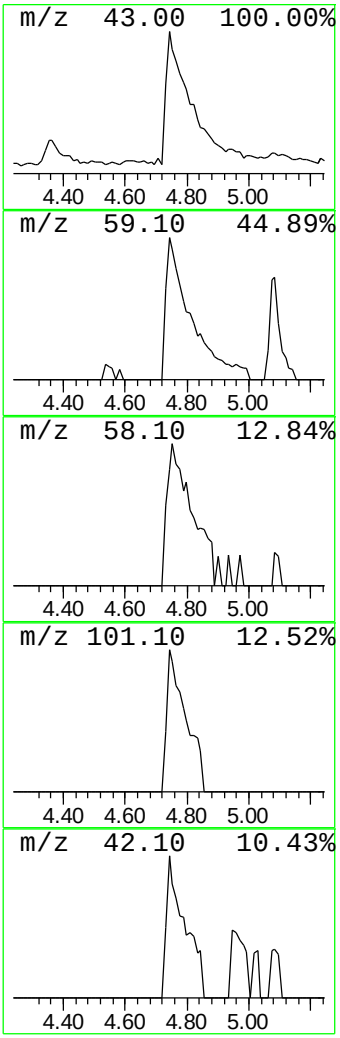
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	3.20 ng	111590	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Diacetamide	101	C4H7NO2	000625-77-4	45
3	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	39
4	2-Pentanone, 5-(2-propynyloxy)-	140	C8H12O2	055702-70-0	25
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

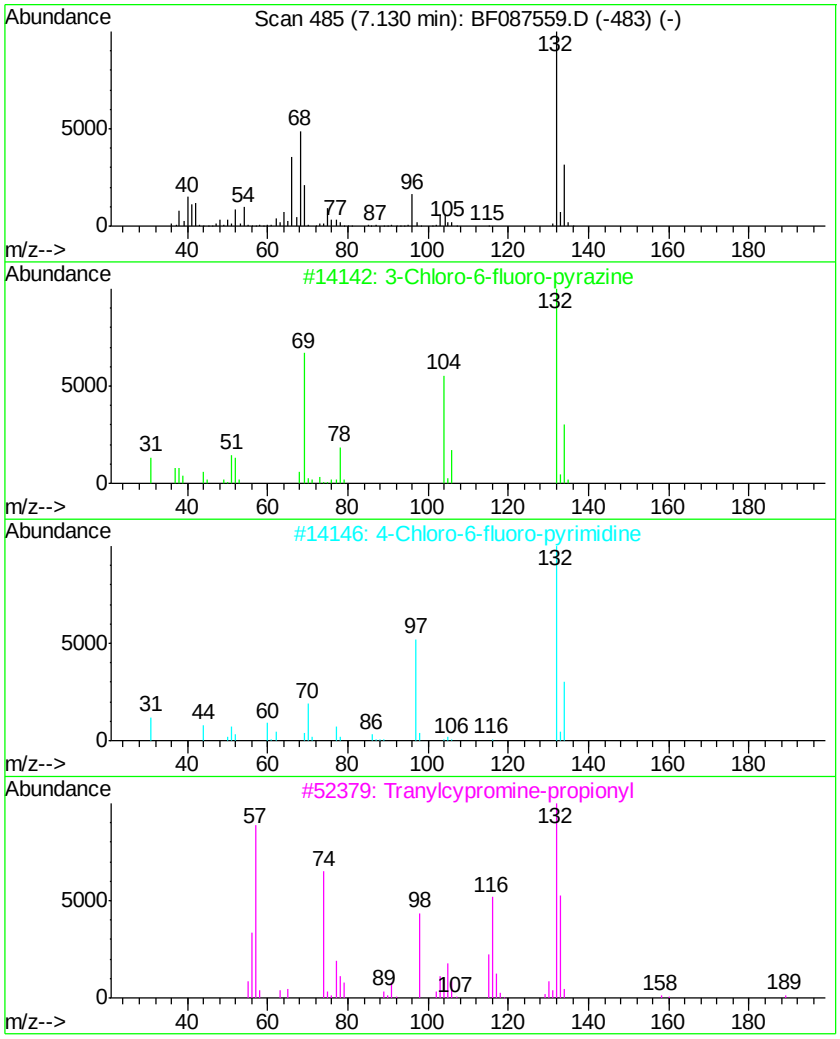
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

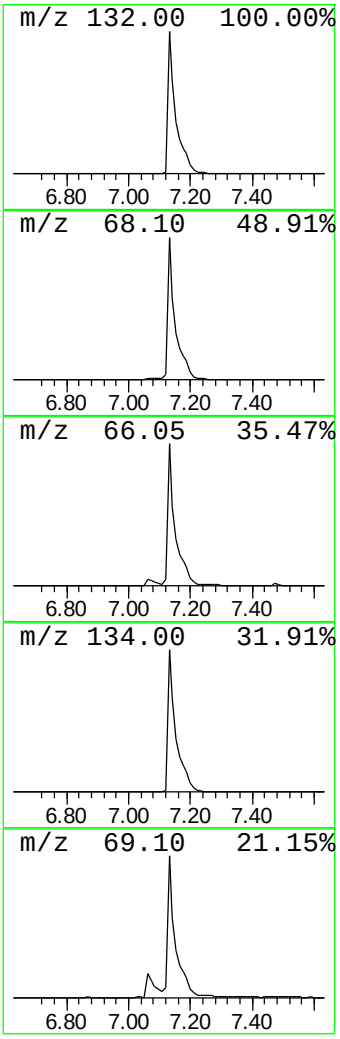
****

Peak Number 5 unknown7.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	81.00 ng	2820680	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

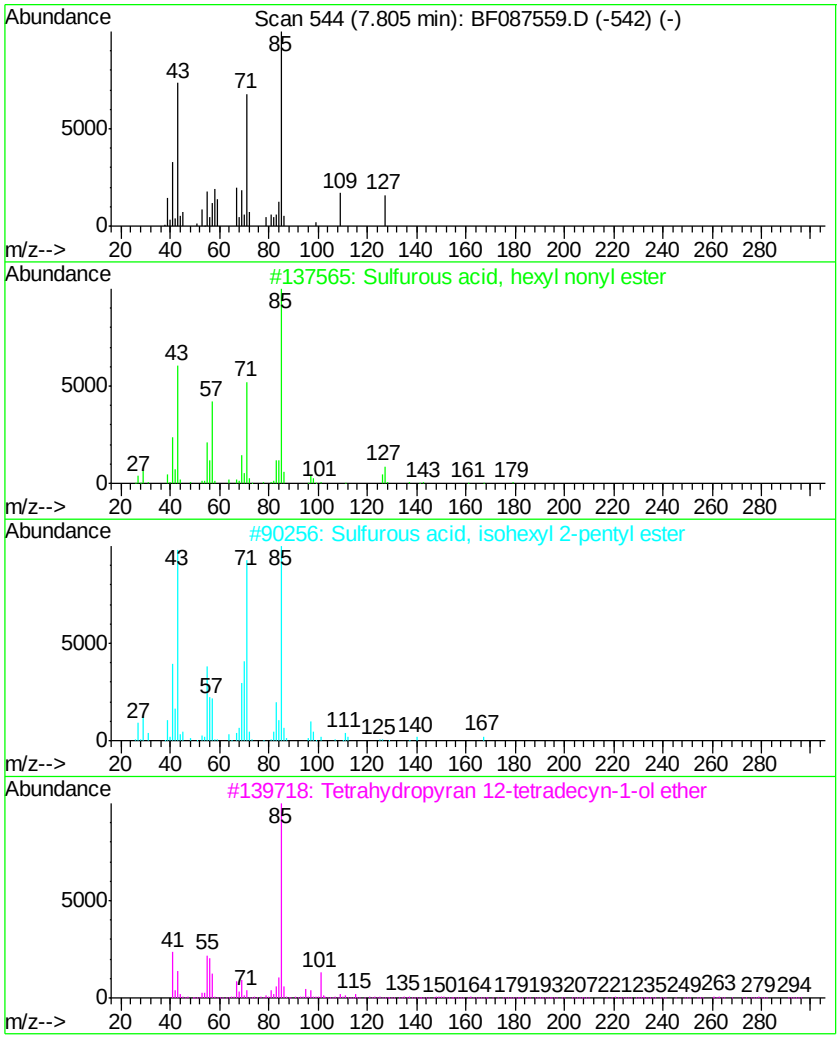
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

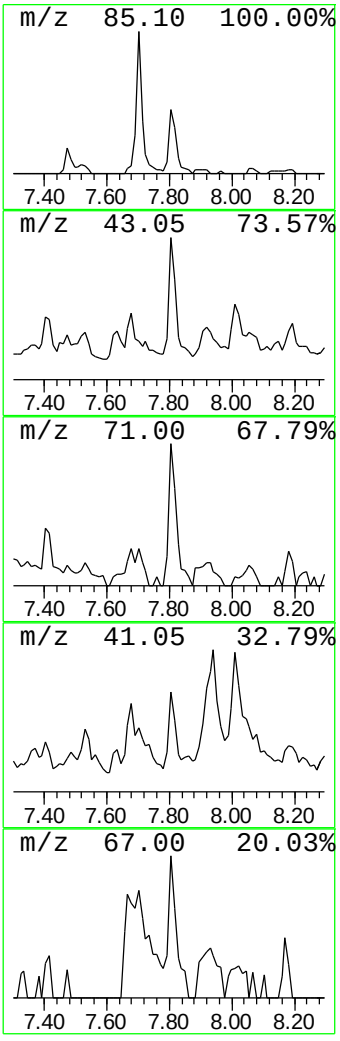
****

Peak Number 7 Sulfurous acid, hexyl nonyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	2.55 ng	88669	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, hexyl nonyl ester	292	C15H32O3S	1000309-13-1	50
2	Sulfurous acid, isohexyl 2-penty...	236	C11H24O3S	1000309-15-5	40
3	Tetrahydropyran 12-tetradecyn-1-...	294	C19H34O2	096249-40-0	38
4	5,6-Epoxyhexanol-1	116	C6H12O2	021915-57-1	37
5	4-Ethyl-4-methyl-1-hexene	126	C9H18	090674-67-2	35





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Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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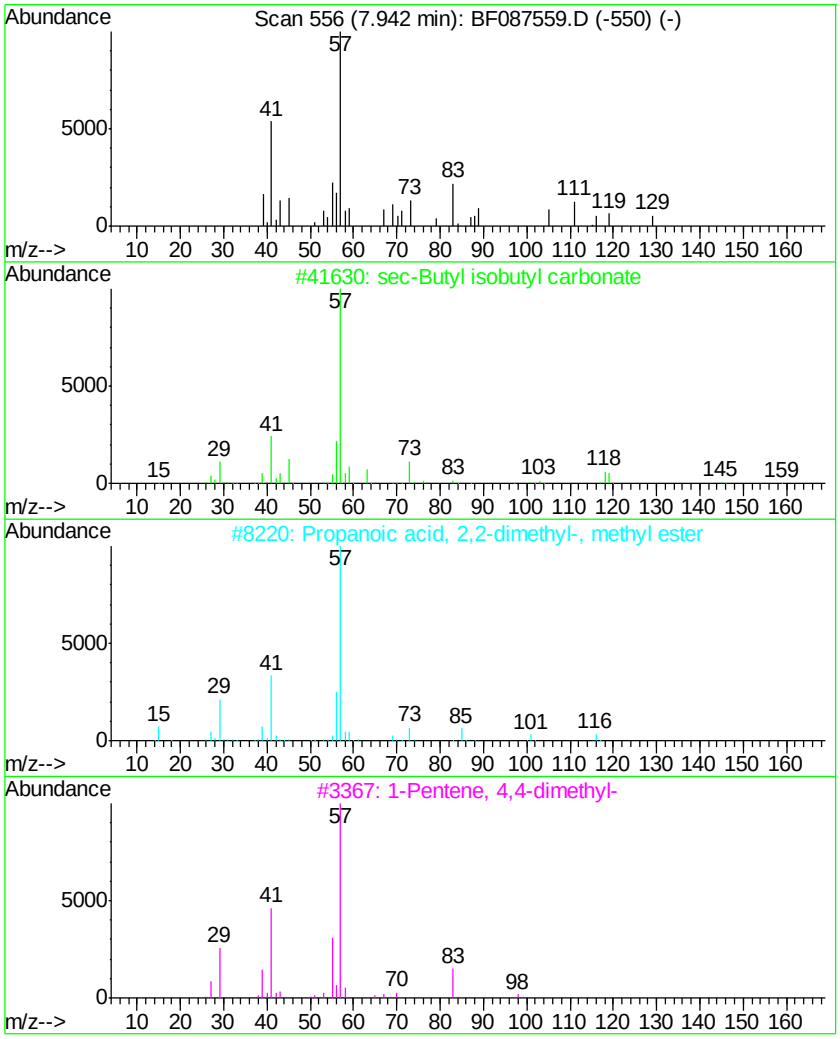
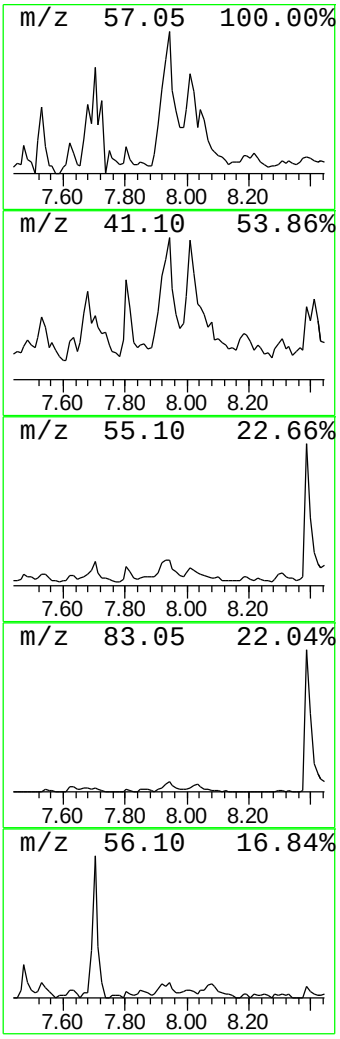
Peak Number 8 unknown7.94 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.94	2.84 ng	98771	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	sec-Butyl isobutyl carbonate	174	C9H18O3	1000372-77-3	25
2	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	17
3	1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	16
4	Propane, 1-(1,1-dimethylethoxy)-...	144	C9H20O	032970-46-0	12
5	1-Isobutoxy-1-methoxypropane	146	C8H18O2	1000245-16-6	12





Library Search Compound Report

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Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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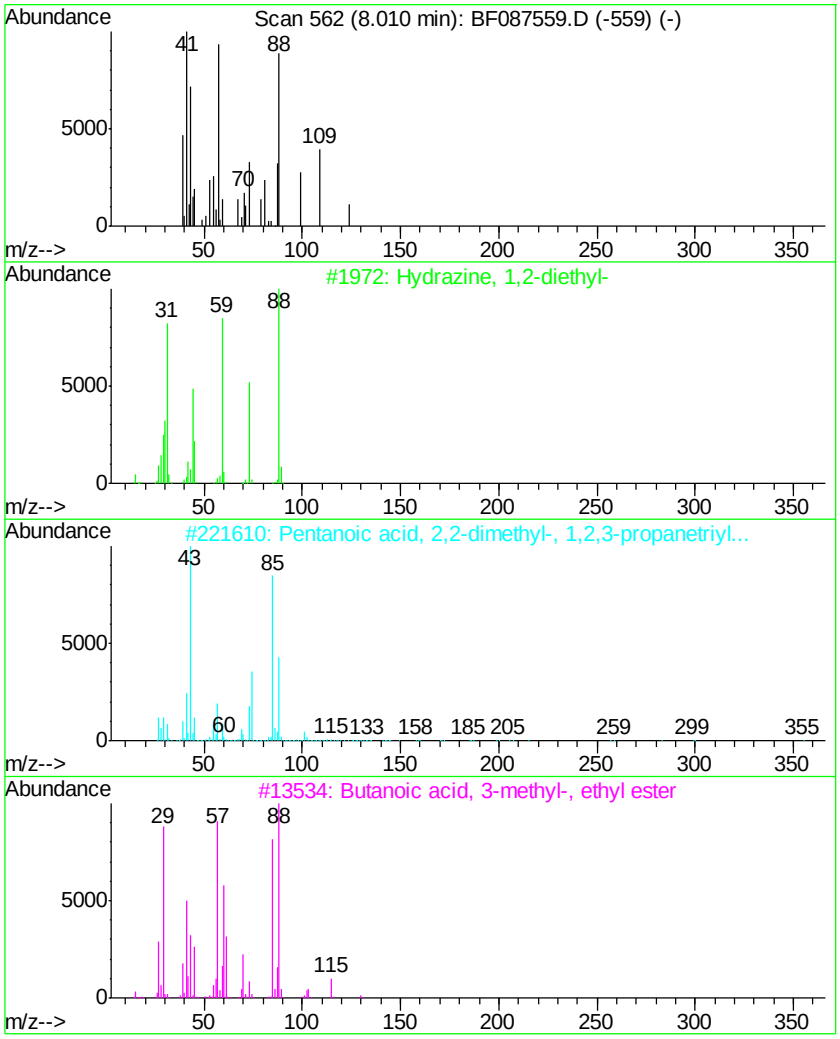
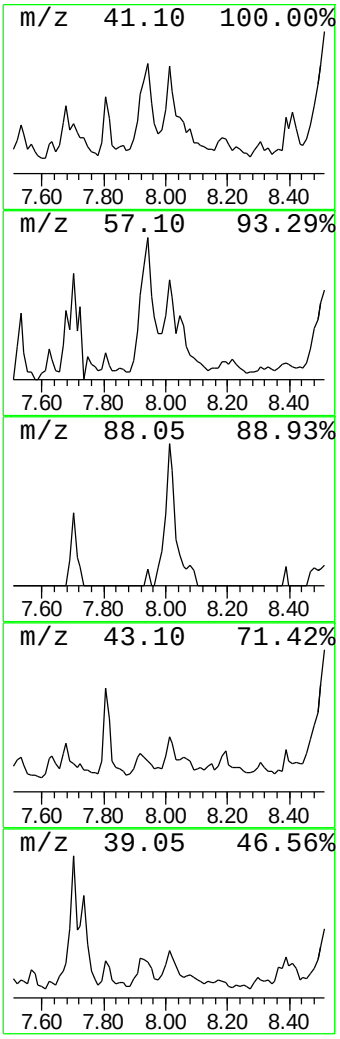
Peak Number 9 unknown8.01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	2.88 ng	100305	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	35
2	Pentanoic acid, 2,2-dimethyl-, 1...	428	C24H44O6	057346-62-0	32
3	Butanoic acid, 3-methyl-, ethyl ...	130	C7H14O2	000108-64-5	32
4	Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	32
5	2,2-Dimethylthiirane	88	C4H8S	003772-13-2	25





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Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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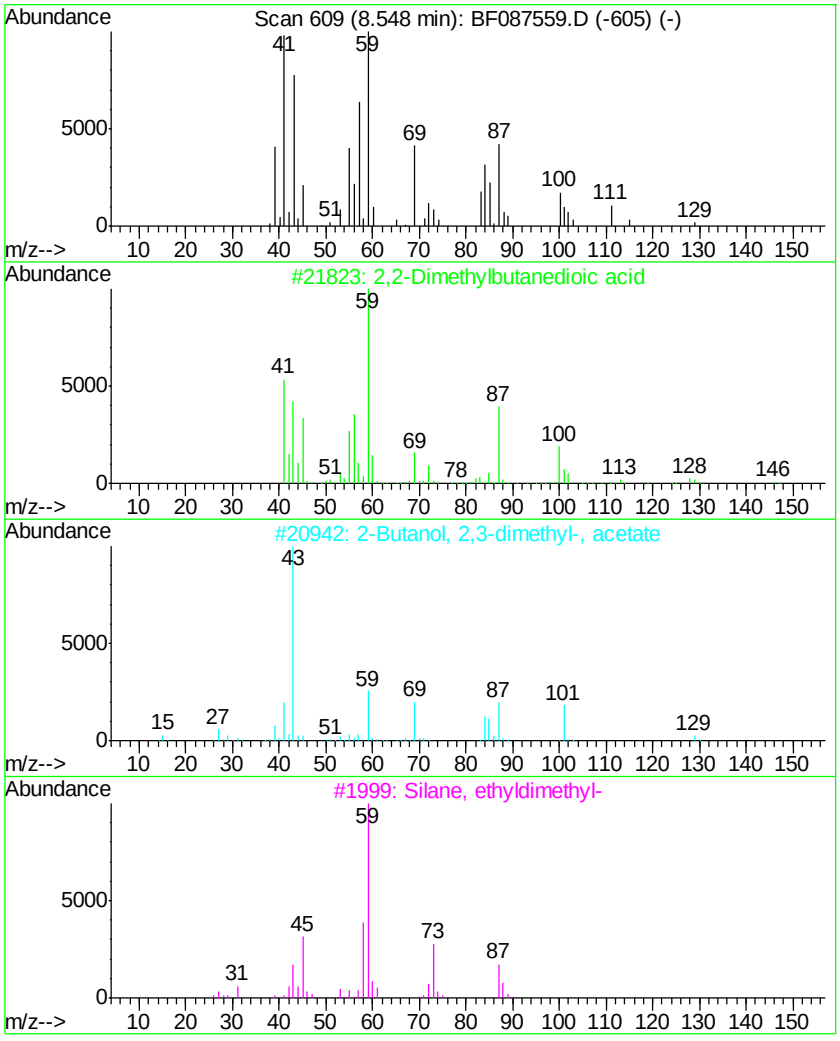
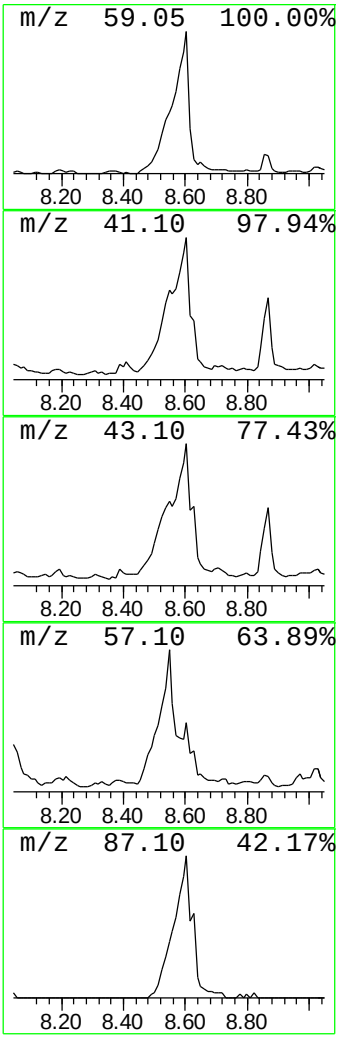
Peak Number 10 2,2-Dimethylbutanedioic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.55	6.75 ng	317311	Naphthalene-d8	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylbutanedioic acid	146	C6H10O4	000597-43-3	59
2	2-Butanol, 2,3-dimethyl-, acetate	144	C8H16O2	004806-33-1	37
3	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	35
4	Allyldimethylsilane	100	C5H12Si	003937-30-2	32
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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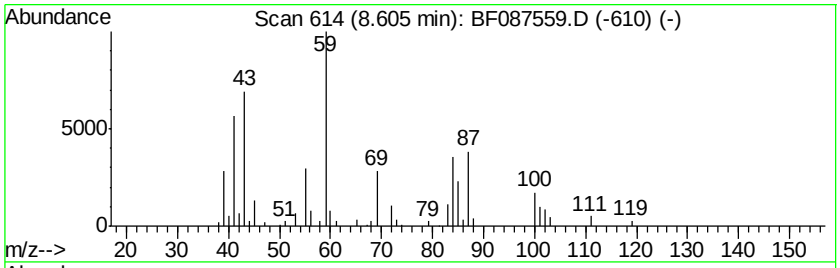
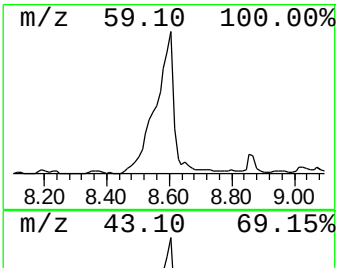
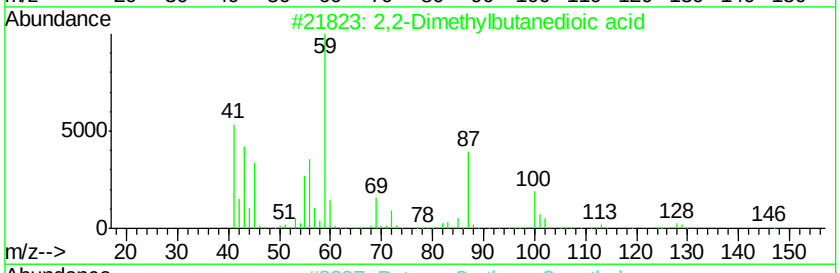
Peak Number 11 unknown8.60 Concentration Rank 3

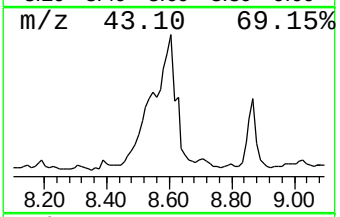
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.60	12.02 ng	564666	Naphthalene-d8	9.51

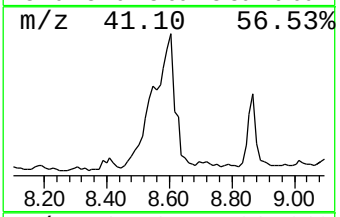
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylbutanedioic acid	146	C6H10O4	000597-43-3	45
2	Butane, 2-ethoxy-2-methyl-	116	C7H16O	000919-94-8	40
3	Allyldimethylsilane	100	C5H12Si	003937-30-2	37
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27
5	Acetaldehyde N-formyl-N-methylhy...	100	C4H8N2O	016568-02-8	25

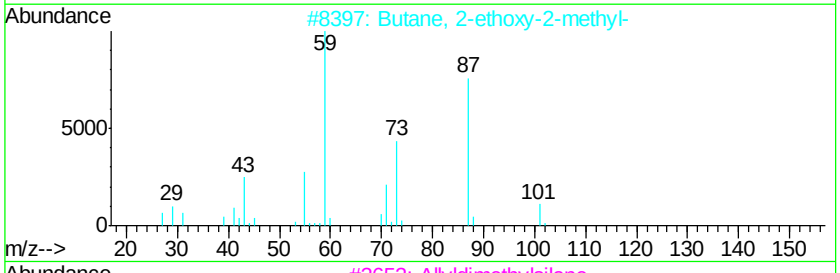


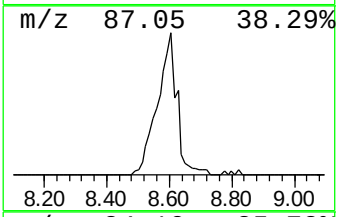


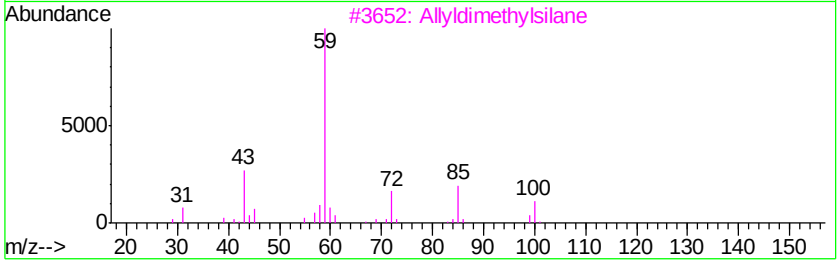


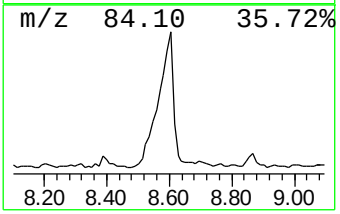












Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

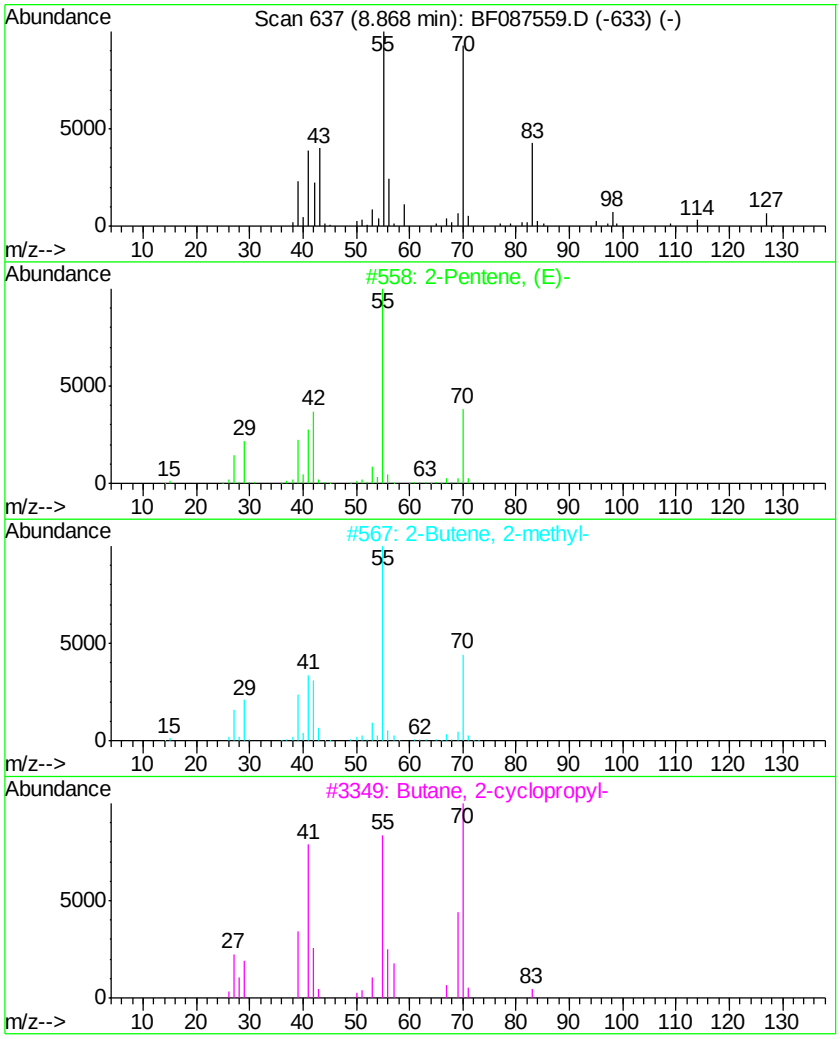
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

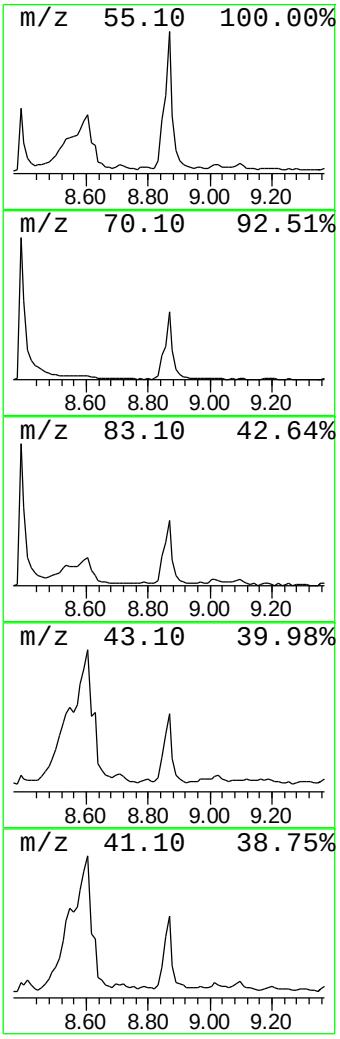
****

Peak Number 12 unknown8.87 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.87	5.45 ng	255971	Naphthalene-d8	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	47
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	47
3	Butane, 2-cyclopropyl-	98	C7H14	005750-02-7	42
4	Heptane, 3-methylene-	112	C8H16	001632-16-2	40
5	Isopropylcyclobutane	98	C7H14	000872-56-0	40





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
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Operator : UM/SJ
Sample : H3317-14
Misc :
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Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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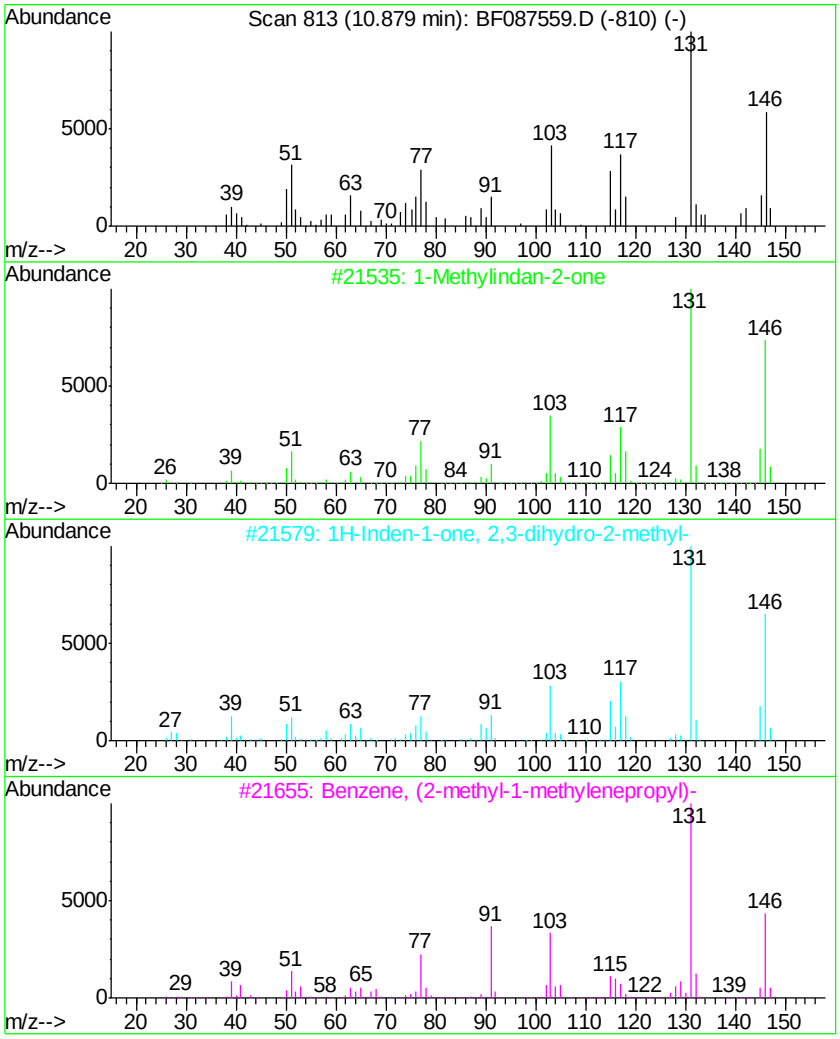
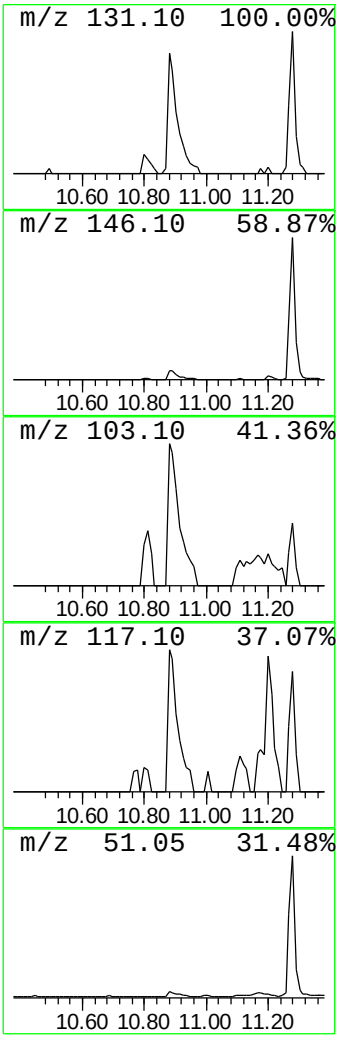
Peak Number 13 1-Methylindan-2-one Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.68 ng	125761	Naphthalene-d8	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylindan-2-one	146	C10H10O	035587-60-1	96
2	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	94
3	Benzene, (2-methyl-1-methylenepr...	146	C11H14	017498-71-4	76
4	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	72
5	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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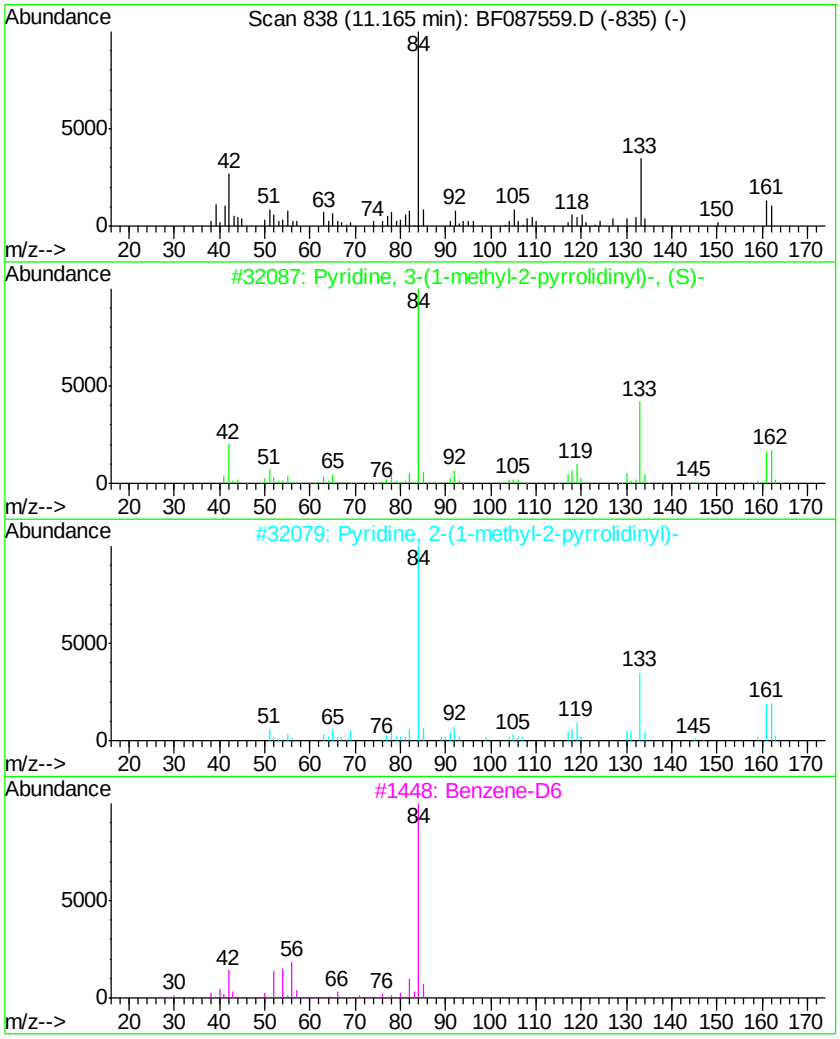
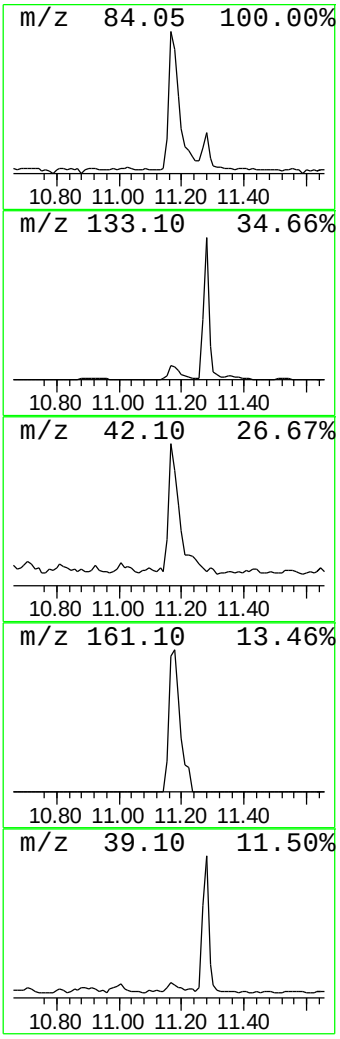
Peak Number 14 Pyridine, 3-(1-methyl-2-pyr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	3.44 ng	170733	Acenaphthene-d10	12.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 3-(1-methyl-2-pyrrolid...	162	C10H14N2	000054-11-5	87
2	Pyridine, 2-(1-methyl-2-pyrrolid...	162	C10H14N2	023950-04-1	86
3	Benzene-D6	84	C6D6	001076-43-3	46
4	2-Oxo-6-(piperidine-1-sulfonyl)-...	388	C15H17ClN2O6S	1000278-11-9	38
5	Pyridine-D5-	84	C5D5N	007291-22-7	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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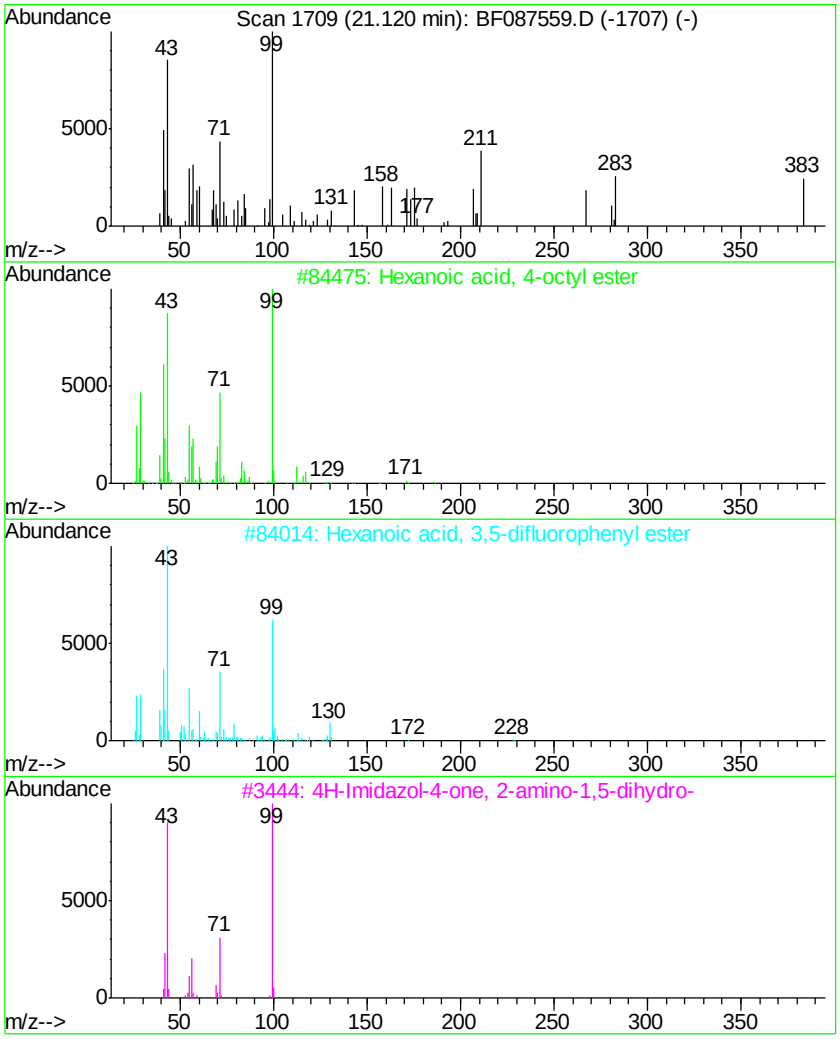
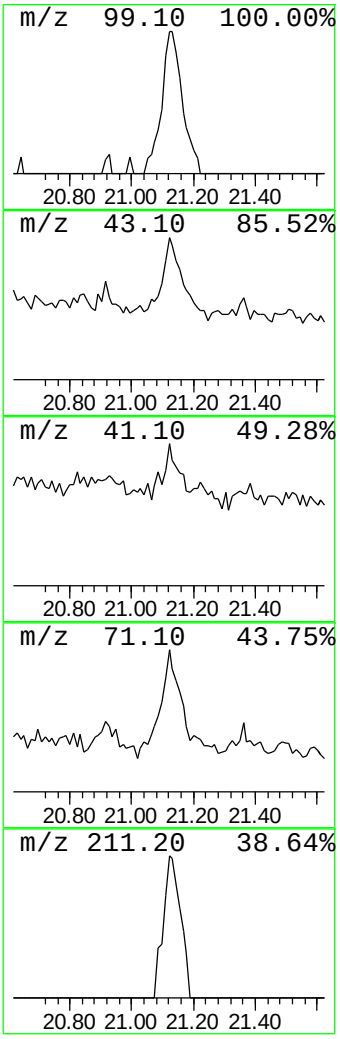
Peak Number 15 unknown21.12 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.12	2.74 ng	77020	Perylene-d12	20.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 4-octyl ester	228	C14H28O2	1000160-13-3	27
2	Hexanoic acid, 3,5-difluorophenyl...	228	C12H14F2O2	1000293-61-4	27
3	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	27
4	3-Dodec-7-enyl-2,4,10-trioxa-ada...	308	C19H32O3	1000193-13-9	16
5	Hexanoic acid, 5-tetradecyl ester	312	C20H40O2	1000279-29-9	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087559.D
Acq On : 30 May 2016 19:56
Operator : UM/SJ
Sample : H3317-14
Misc :
ALS Vial : 79 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GMW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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-Butanol, 2,3-di...	2.18	2.7	ng	95329	1	7.47	696450	20.0
2-Pentanone, 4-hy...	4.74	3.2	ng	111590	1	7.47	696450	20.0
unknown7.13	7.13	81.0	ng	2820680	1	7.47	696450	20.0
Sulfurous acid, h...	7.80	2.5	ng	88669	1	7.47	696450	20.0
unknown7.94	7.94	2.8	ng	98771	1	7.47	696450	20.0
unknown8.01	8.01	2.9	ng	100305	1	7.47	696450	20.0
2,2-Dimethylbutan...	8.55	6.8	ng	317311	2	9.51	939897	20.0
unknown8.60	8.60	12.0	ng	564666	2	9.51	939897	20.0
unknown8.87	8.87	5.5	ng	255971	2	9.51	939897	20.0
1-Methylindan-2-one	10.88	2.7	ng	125761	2	9.51	939897	20.0
Pyridine, 3-(1-me...	11.16	3.4	ng	170733	3	12.33	991706	20.0
unknown21.12	21.12	2.7	ng	77020	6	20.15	562917	20.0