LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062918\
Data File : BG035510.D
Acq On : 29 Jun 2018 12:20
Operator : JU/SJ
Sample : J3593-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S39-9005

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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	4.262	161	166	172	rBV	28277	43696	1.47%	0.346%
2	5.173	314	321	330	rBV	212319	319824	10.77%	2.536%
3	5.637	394	400	408	rBV	271037	434125	14.63%	3.443%
4	7.223	662	670	681	rBV	626525	1079347	36.36%	8.559%
5	7.599	725	734	744	rBV	439772	770123	25.94%	6.107%
6	8.063	806	813	819	rBV2	97866	167971	5.66%	1.332%
7	8.386	860	868	876	rVB	465629	794214	26.76%	6.298%
8	9.220	1002	1010	1019	rBV	390486	719425	24.24%	5.705%
9	10.865	1283	1290	1299	rBV	134021	240961	8.12%	1.911%
10	13.309	1699	1706	1719	rBV	1138603	1828465	61.60%	14.499%
11	14.126	1838	1845	1854	rBV	128983	194698	6.56%	1.544%
12	14.684	1932	1940	1949	rBV	249092	400090	13.48%	3.173%
13	16.164	2185	2192	2200	rBV	299670	479274	16.15%	3.801%
14	16.375	2224	2228	2236	rBV3	22209	38986	1.31%	0.309%
15	17.168	2356	2363	2367	rBV3	19155	30043	1.01%	0.238%
16	17.421	2400	2406	2412	rBV	372208	578874	19.50%	4.590%
17	18.302	2552	2556	2561	rBV5	35639	48231	1.62%	0.382%
18	19.835	2813	2817	2822	rVB6	21441	31653	1.07%	0.251%
19	20.029	2844	2850	2857	rVB	2271005	2968307	100.00%	23.538%
20	21.322	3067	3070	3075	rVB3	54679	79182	2.67%	0.628%
21	21.568	3110	3112	3119	rVB5	34061	49149	1.66%	0.390%
22	21.686	3127	3132	3140	rBV2	374328	637354	21.47%	5.054%
23	23.372	3415	3419	3423	rBV3	35307	51742	1.74%	0.410%
24	24.917	3673	3682	3697	rVB	207480	624988	21.06%	4.956%

Sum of corrected areas: 12610722

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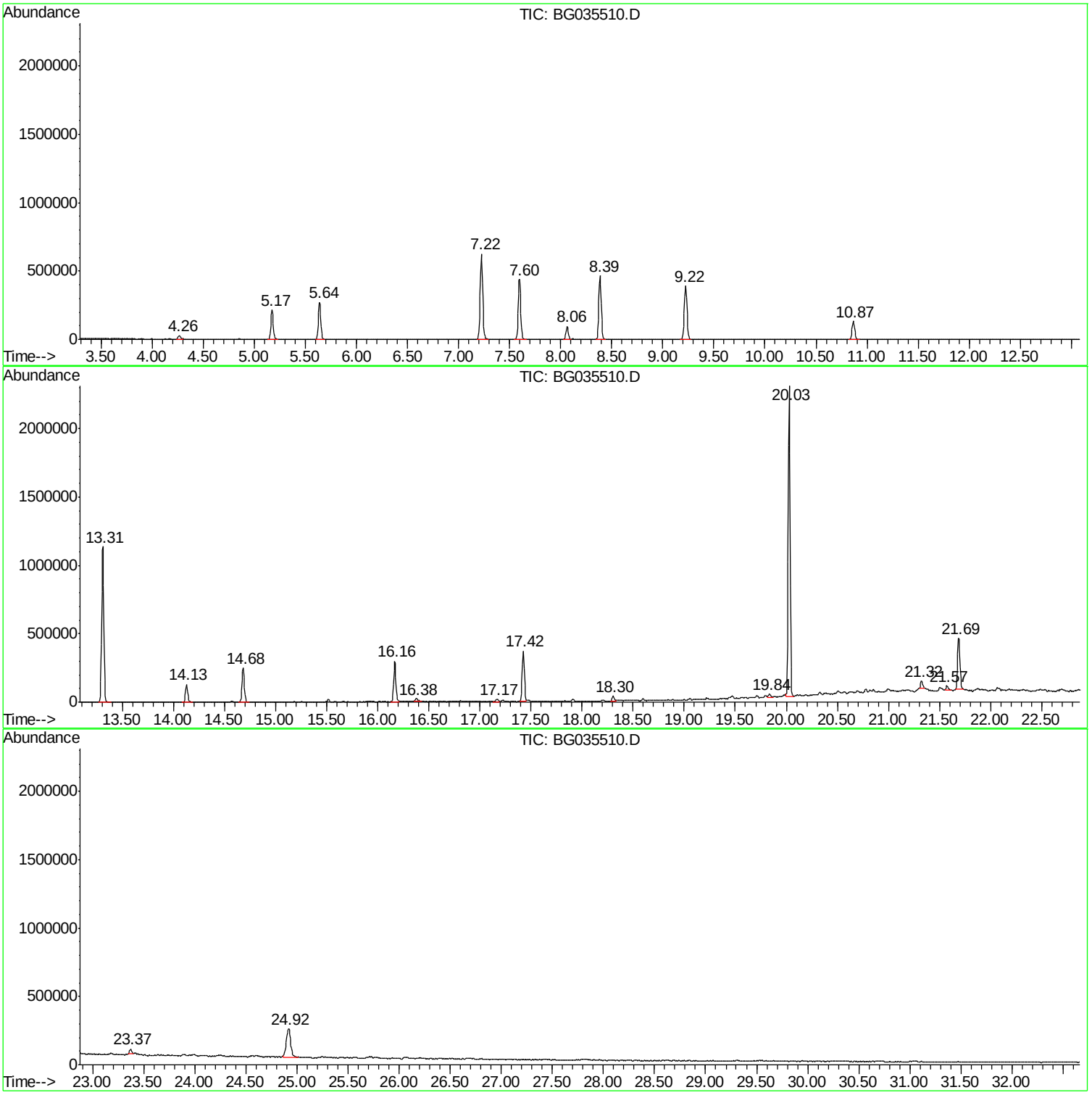
Instrument :
BNA_G
ClientSampleId :
S39-9005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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

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TIC Integration Parameters: LSCINT.P

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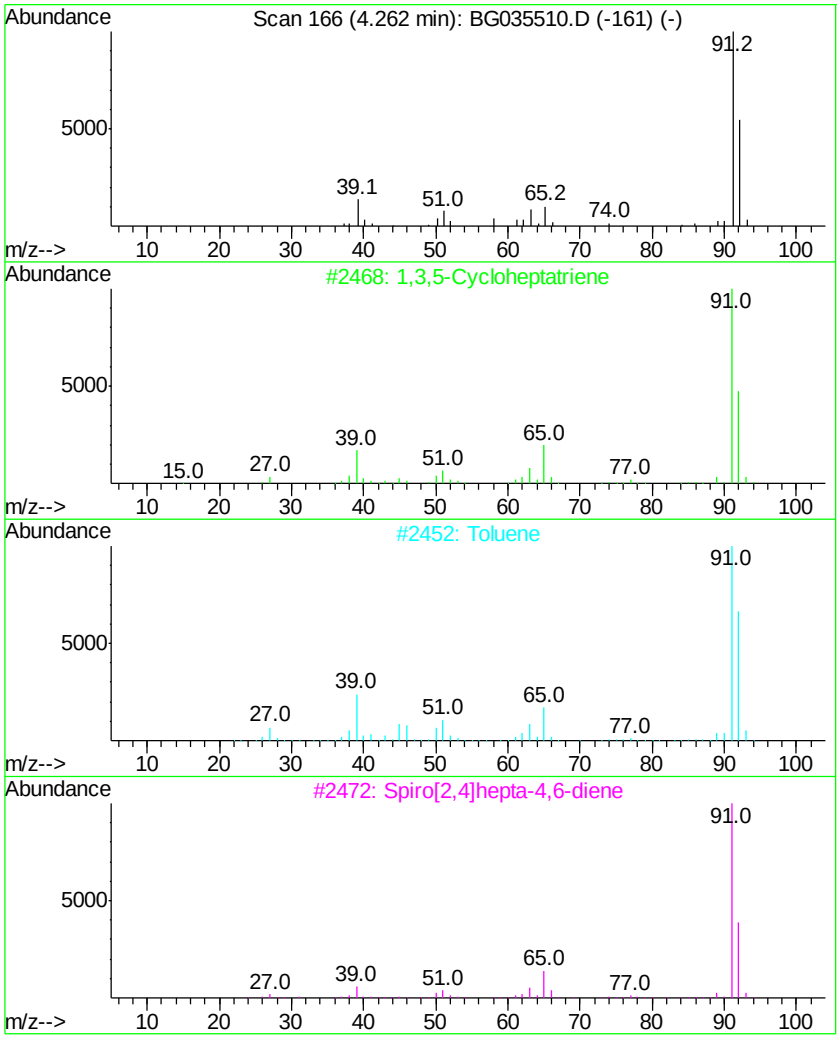
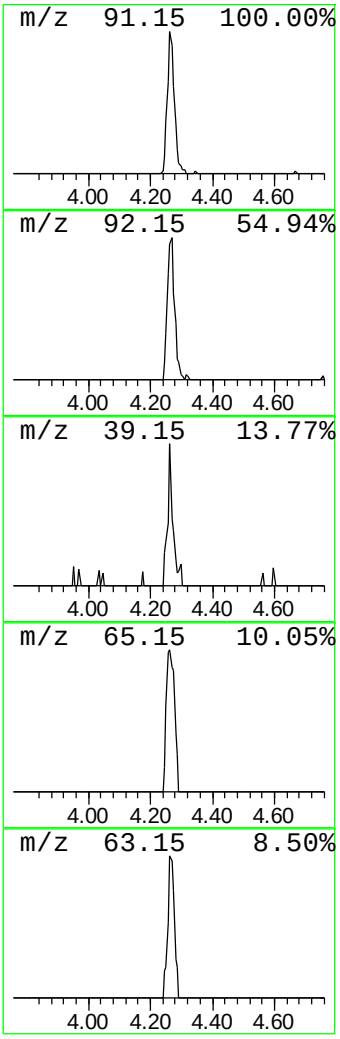
Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	5.20 ng	43696	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
2	Toluene	92	C7H8	000108-88-3	87
3	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	86
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	78
5	Tetracyclo[3.2.0.0(2,7).0(4,6)]h...	92	C7H8	000278-06-8	64





Library Search Compound Report

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Operator : JU/SJ
Sample : J3593-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S39-9005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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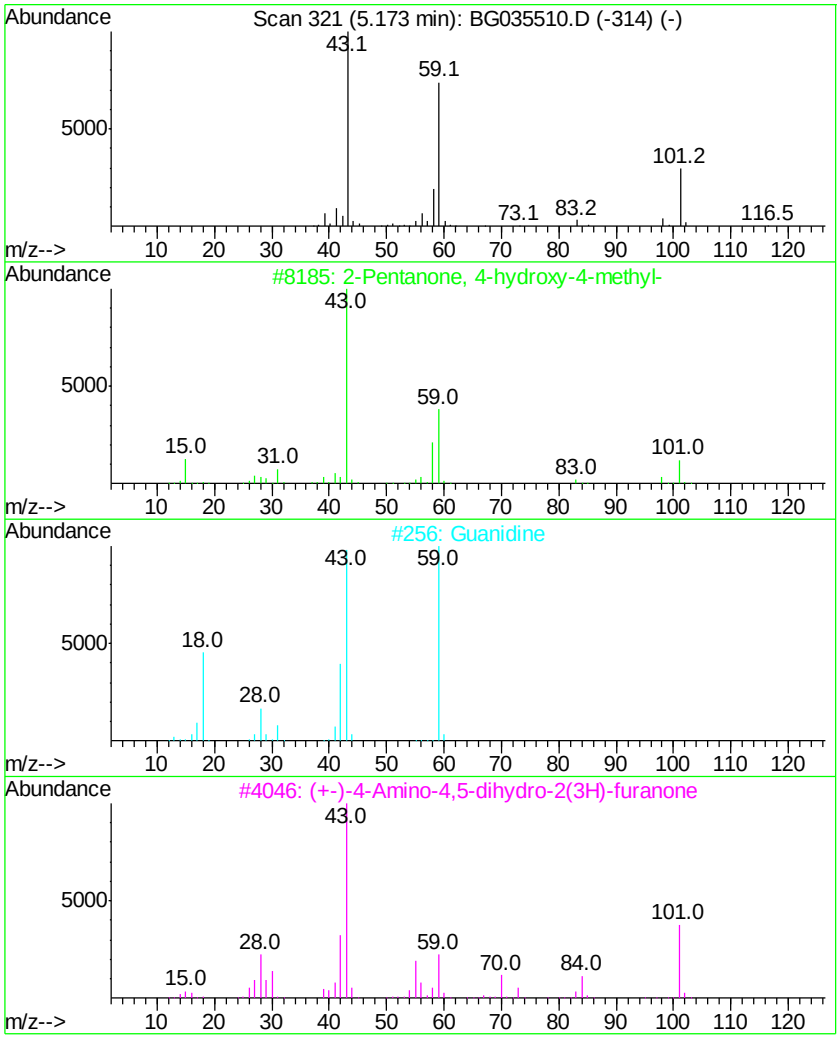
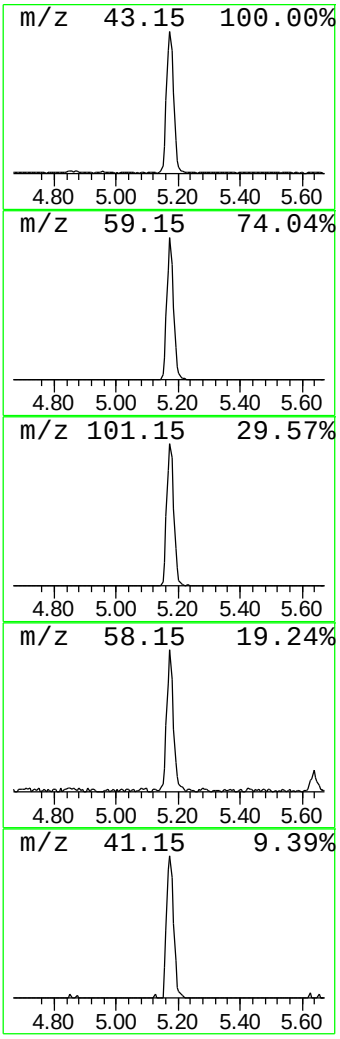
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	38.08 ng	319824	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Guanidine	59	CH5N3	000113-00-8	47
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

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Data File : BG035510.D
Acq On : 29 Jun 2018 12:20
Operator : JU/SJ
Sample : J3593-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S39-9005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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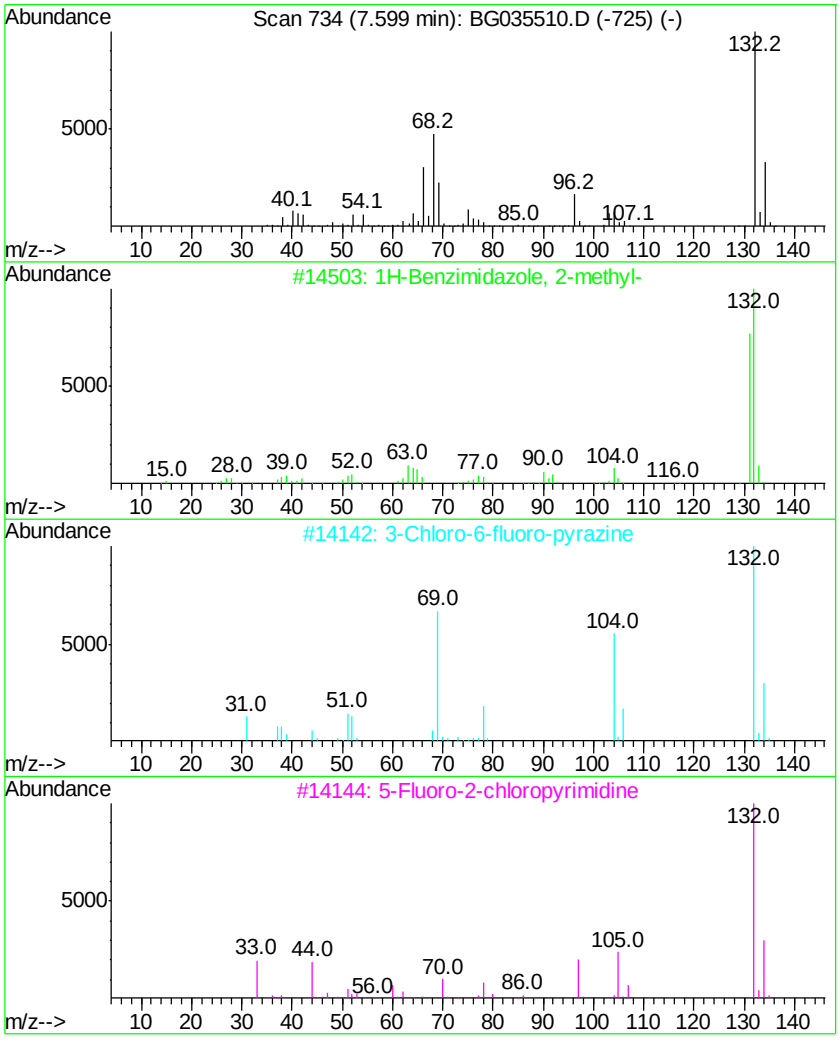
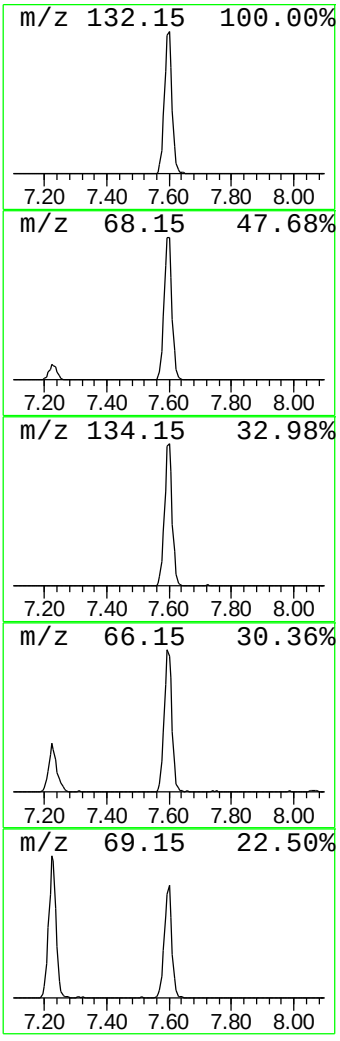
Peak Number 3 unknown7.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	91.70 ng	770123	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	1H-Indazole, 3-methyl-	132	C8H8N2	1000316-00-2	12
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





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Sample : J3593-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S39-9005

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
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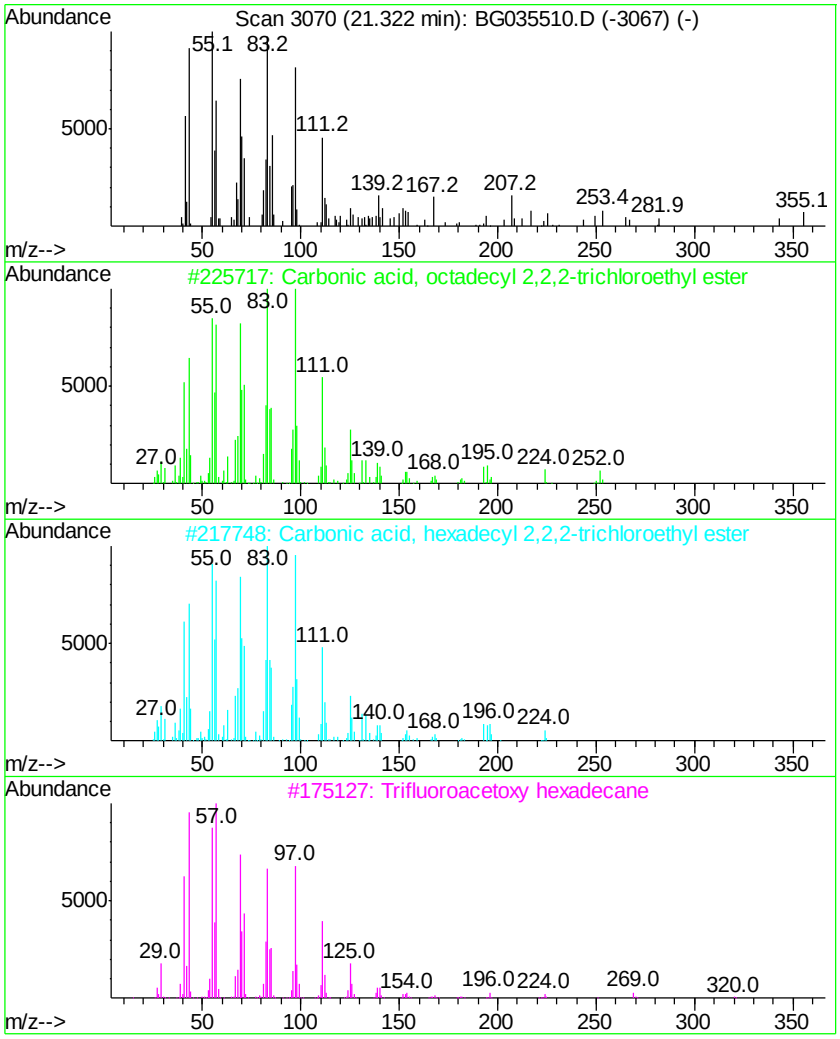
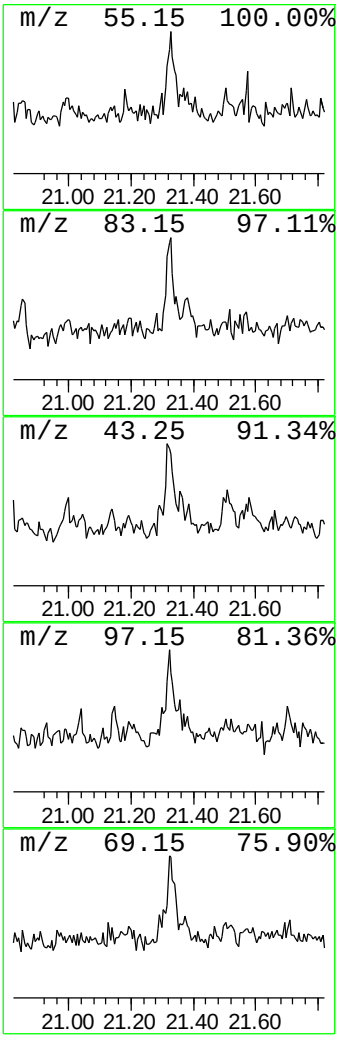
Peak Number 5 Carbonic acid, octadecyl 2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	2.48 ng	79182	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	90
2	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	87
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86
5	1-Heneicosanol	312	C21H44O	015594-90-8	86





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
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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
1,3,5-Cycloheptat...	4.26	5.2	ng	43696	1	8.06	167971	20.0
2-Pentanone, 4-hy...	5.17	38.1	ng	319824	1	8.06	167971	20.0
unknown7.60	7.60	91.7	ng	770123	1	8.06	167971	20.0
Carbonic acid, oc...	21.32	2.5	ng	79182	5	21.69	637354	20.0