LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090119\
Data File : BG042678.D
Acq On : 2 Sep 2019 1:42
Operator : HP/JU
Sample : K4554-39
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8-(0-2)

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-BG082219.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	3.114	3	4	18	rVB	101825	129387	6.71%	1.555%
2	4.471	230	235	243	rBV	37694	54222	2.81%	0.652%
3	5.076	332	338	347	rBV	120252	183619	9.53%	2.206%
4	5.552	413	419	432	rVB	127132	213687	11.09%	2.568%
5	7.162	686	693	704	rBV	267390	495701	25.72%	5.956%
6	7.526	748	755	768	rBV	245213	427101	22.16%	5.132%
7	7.996	827	835	843	rBV	89669	150047	7.79%	1.803%
8	8.325	883	891	902	rVB	247250	443519	23.02%	5.329%
9	9.165	1025	1034	1045	rBV	159705	309185	16.04%	3.715%
10	10.822	1307	1316	1334	rBV	98999	203811	10.58%	2.449%
11	13.272	1725	1733	1748	rBV	560379	961090	49.87%	11.548%
12	14.107	1869	1875	1887	rBV	37293	78413	4.07%	0.942%
13	14.653	1962	1968	1983	rBV2	195129	334433	17.35%	4.018%
14	16.157	2218	2224	2240	rBV2	76783	159867	8.30%	1.921%
15	17.409	2430	2437	2451	rBV2	279097	483057	25.07%	5.804%
16	19.829	2845	2849	2856	rVB	13745	19917	1.03%	0.239%
17	20.017	2875	2881	2892	rBV	1428764	1927015	100.00%	23.155%
18	20.816	3011	3017	3020	rBV	16596	20158	1.05%	0.242%
19	21.316	3097	3102	3114	rBV	49582	96069	4.99%	1.154%
20	21.680	3156	3164	3182	rVB	373353	656615	34.07%	7.890%
21	21.874	3191	3197	3204	rBV	18973	28592	1.48%	0.344%
22	22.479	3295	3300	3307	rBV2	21730	37718	1.96%	0.453%
23	23.178	3411	3419	3424	rBV3	31726	60981	3.16%	0.733%
24	23.989	3549	3557	3565	rVB2	32035	68445	3.55%	0.822%
25	24.923	3704	3716	3736	rBV2	222219	735138	38.15%	8.833%
26	26.087	3905	3914	3923	rVB6	14697	44557	2.31%	0.535%

Sum of corrected areas: 8322344

LSC Report - Integrated Chromatogram

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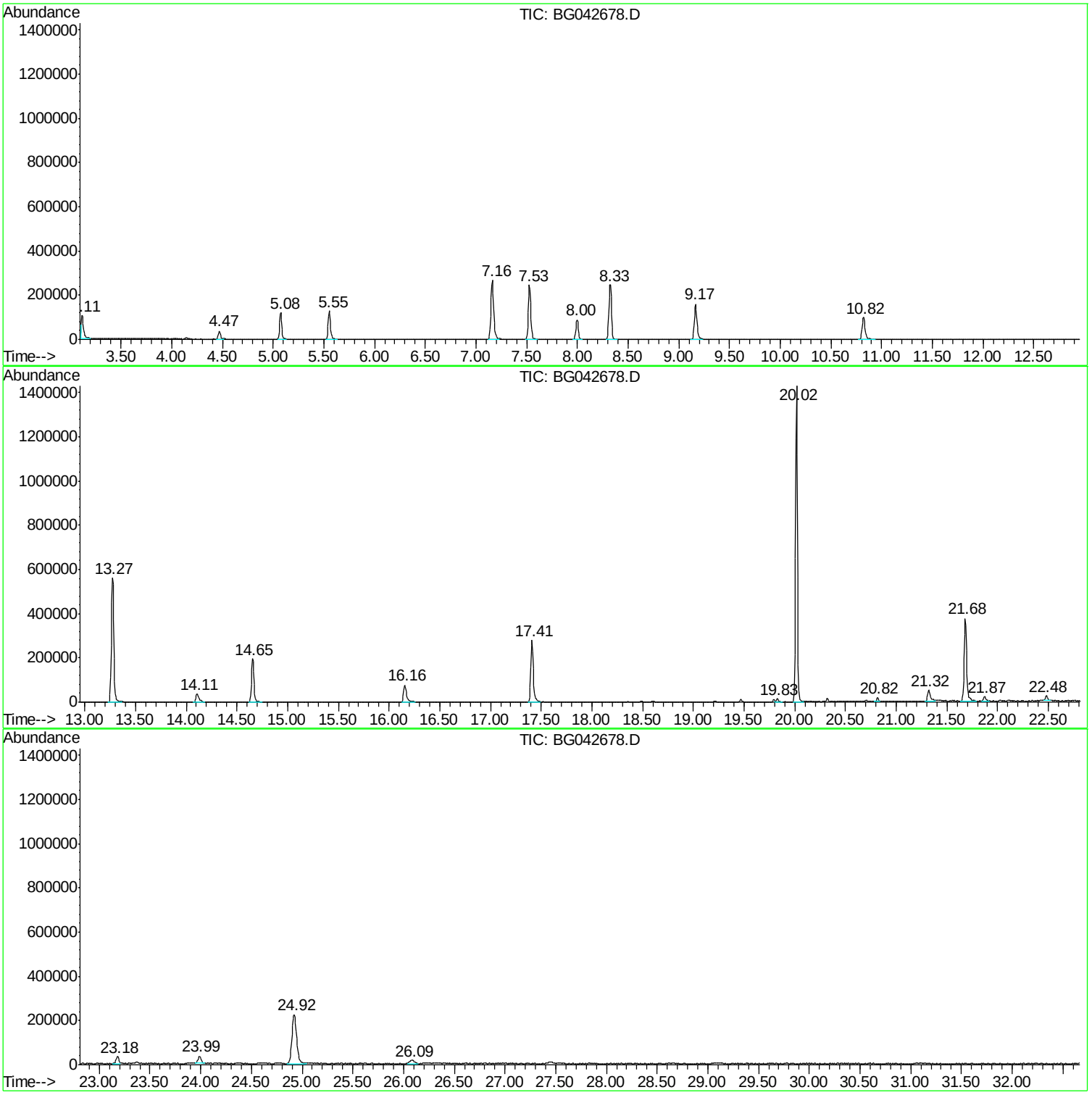
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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:\SVOASRV\HPCHEM1\BNA G\DATA\BG090119\
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Operator : HP/JU
Sample : K4554-39
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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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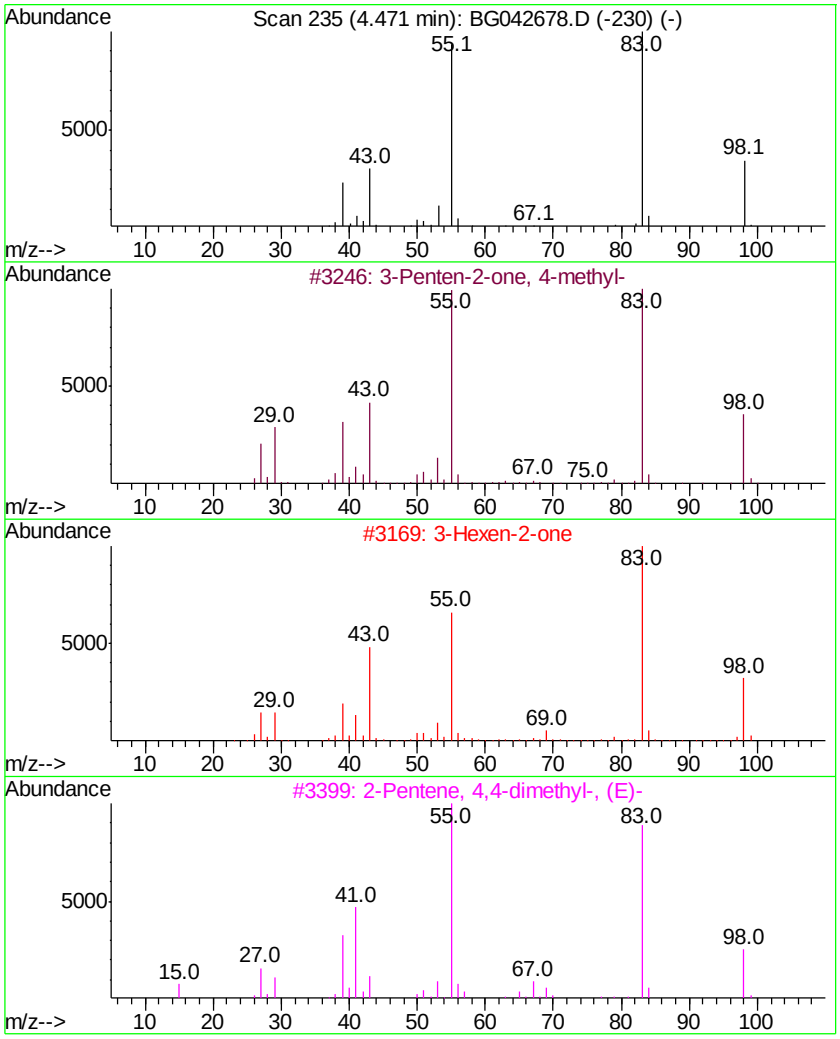
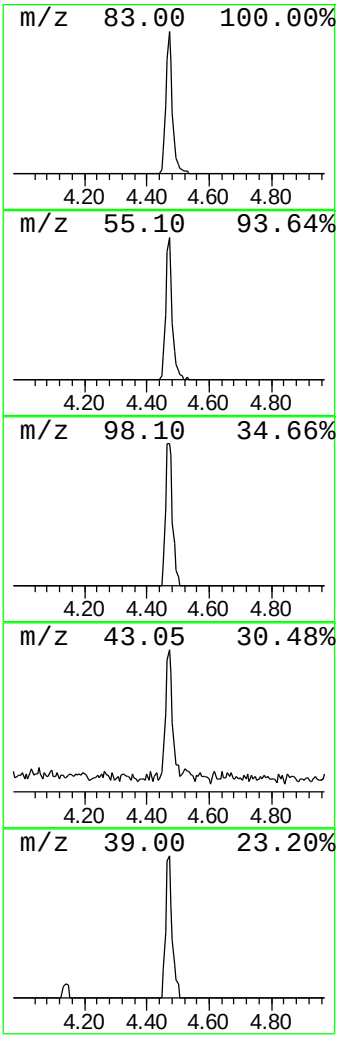
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	7.23 ng	54222	1,4-Dichlorobenzene-d4	8.00

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	90
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86





Library Search Compound Report

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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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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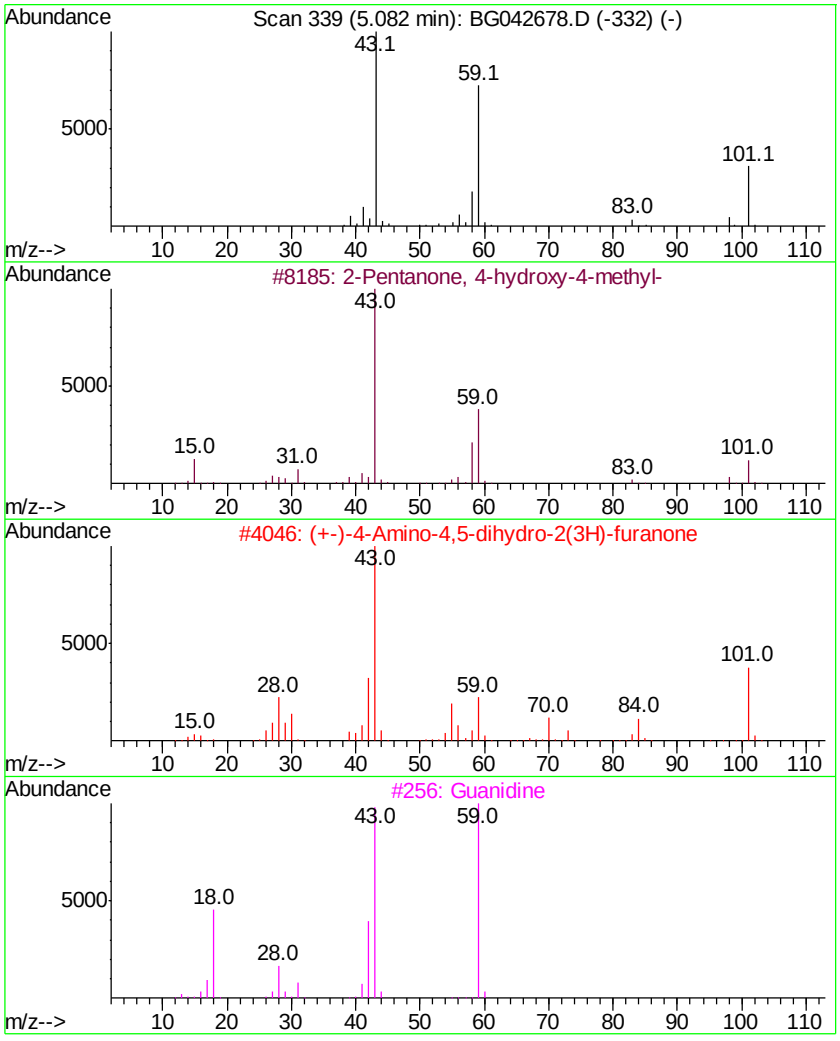
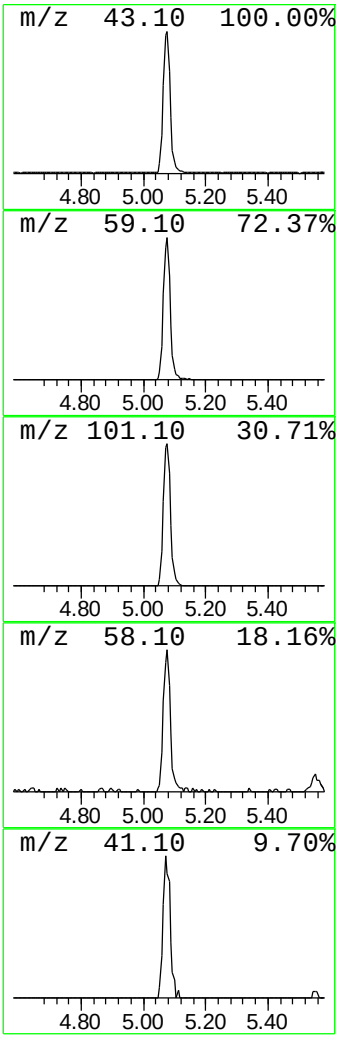
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	24.47 ng	183619	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Guanidine	59	CH5N3	000113-00-8	43
4	1,2-Butanediol	90	C4H10O2	000584-03-2	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Data File : BG042678.D
Acq On : 2 Sep 2019 1:42
Operator : HP/JU
Sample : K4554-39
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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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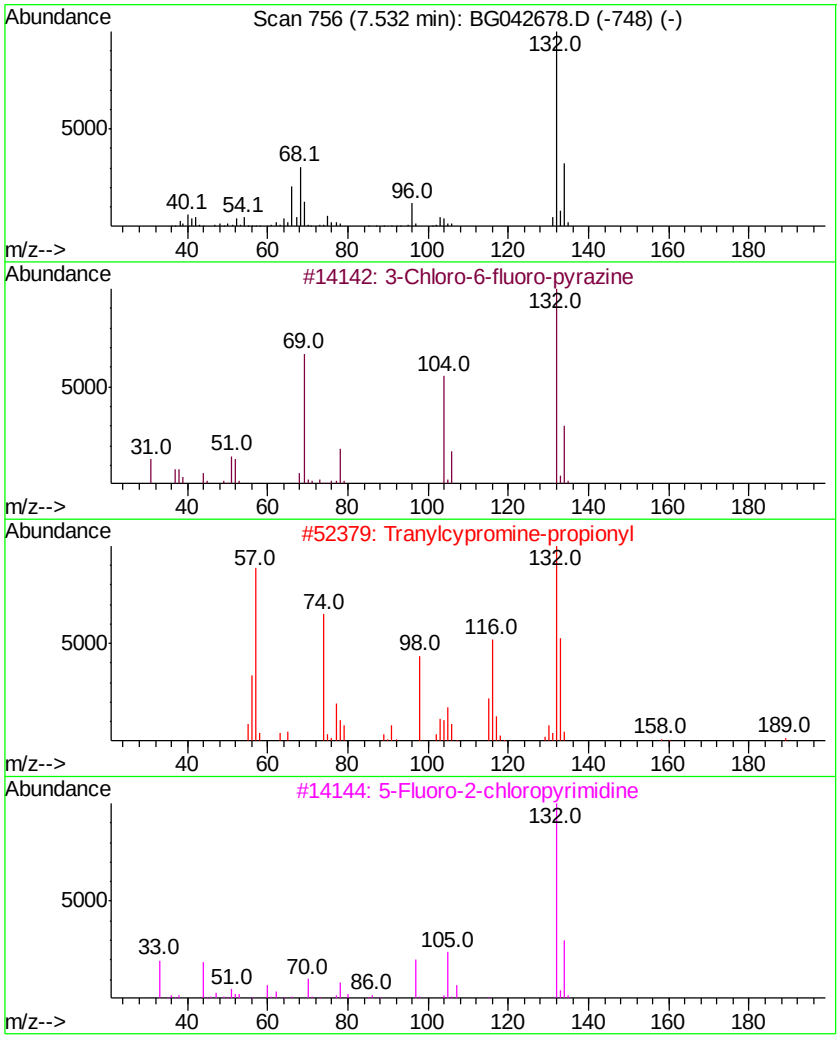
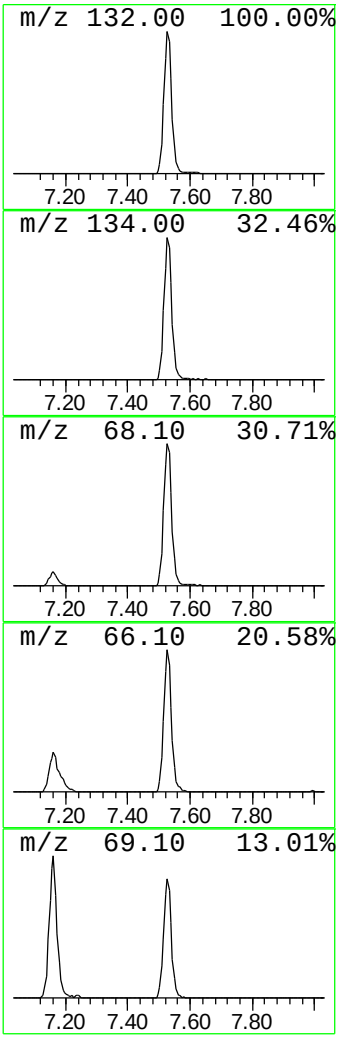
Peak Number 4 unknown7.53 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	56.93 ng	427101	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Sample : K4554-39
Misc :
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Instrument : BNA_G
ClientSampleId : SB-8-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
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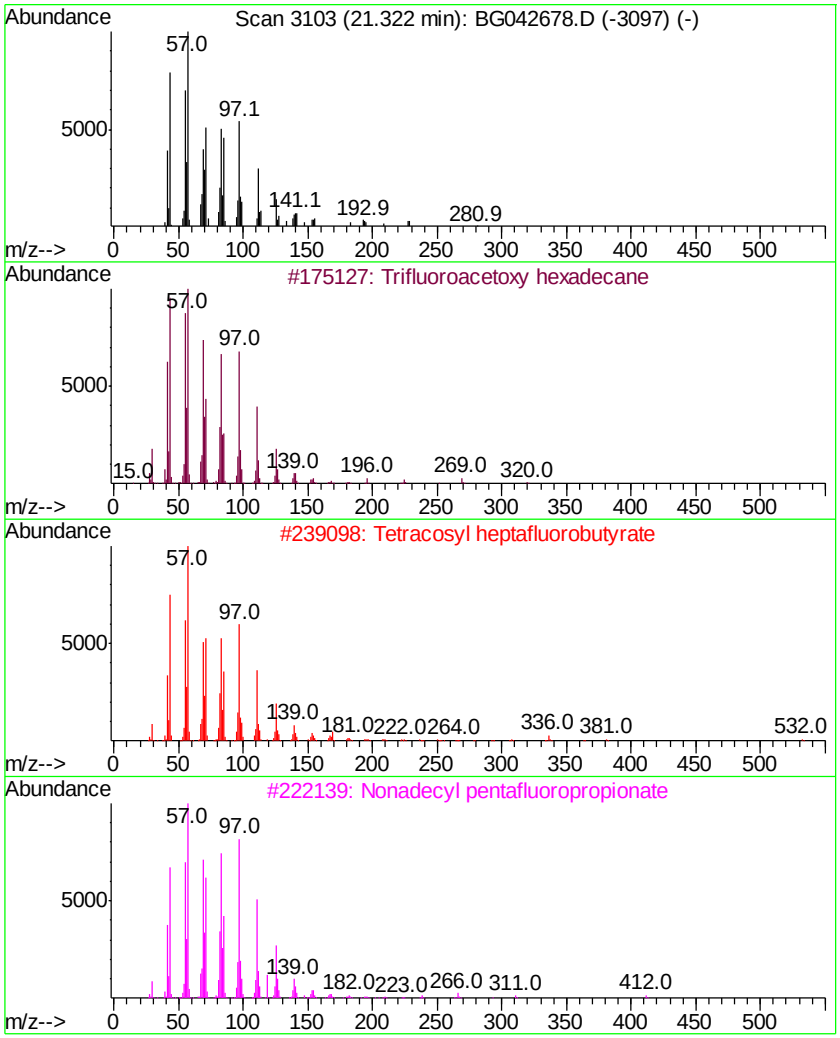
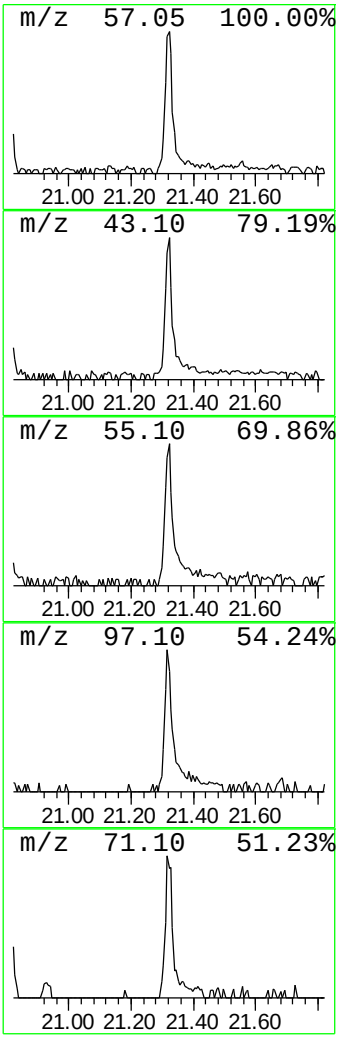
Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	2.93 ng	96069	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG090119\
Data File : BG042678.D
Acq On : 2 Sep 2019 1:42
Operator : HP/JU
Sample : K4554-39
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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
3-Penten-2-one, 4...	4.47	7.2	ng	54222	1	8.00	150047	20.0
2-Pentanone, 4-hy...	5.08	24.5	ng	183619	1	8.00	150047	20.0
unknown7.53	7.53	56.9	ng	427101	1	8.00	150047	20.0
Trifluoroacetoxy ...	21.32	2.9	ng	96069	5	21.68	656615	20.0