LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031119\
Data File : BG039850.D
Acq On : 11 Mar 2019 20:28
Operator : JU/SJ
Sample : K1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MR-MH-11-COMP

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-BG030419.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	3.205	15	20	29	rBV	68551	132439	3.88%	0.735%
2	3.282	29	33	41	rVB	48776	71218	2.09%	0.395%
3	5.696	437	444	455	rBV	808895	1313560	38.51%	7.295%
4	7.300	709	717	731	rBV	870522	1576468	46.22%	8.755%
5	7.681	774	782	797	rBV	814891	1392355	40.82%	7.732%
6	8.157	852	863	872	rVB	137872	240331	7.05%	1.335%
7	8.480	909	918	926	rBV	561725	991354	29.06%	5.505%
8	9.332	1055	1063	1072	rBV	512254	897468	26.31%	4.984%
9	10.977	1335	1343	1351	rBV	194817	346665	10.16%	1.925%
10	13.403	1748	1756	1763	rBV	1382875	2133993	62.56%	11.851%
11	14.220	1888	1895	1903	rBV	75117	110044	3.23%	0.611%
12	14.778	1981	1990	1998	rBV2	337123	533137	15.63%	2.961%
13	16.264	2236	2243	2253	rBV	1196121	1869935	54.82%	10.384%
14	17.521	2450	2457	2463	rBV2	468324	732633	21.48%	4.069%
15	18.373	2597	2602	2612	rBV	41561	72027	2.11%	0.400%
16	20.118	2893	2899	2905	rBV	2649867	3411011	100.00%	18.942%
17	21.398	3113	3117	3125	rBV3	52488	99985	2.93%	0.555%
18	21.809	3180	3187	3194	rBV	502127	875922	25.68%	4.864%
19	21.956	3206	3212	3216	rBV2	28135	37582	1.10%	0.209%
20	22.579	3311	3318	3323	rBV3	31921	54498	1.60%	0.303%
21	23.301	3433	3441	3447	rBV2	38927	76064	2.23%	0.422%
22	24.136	3574	3583	3596	rVB3	37267	86824	2.55%	0.482%
23	25.181	3741	3761	3779	rBV2	275910	899103	26.36%	4.993%
24	26.303	3944	3952	3961	rVB4	18230	52636	1.54%	0.292%

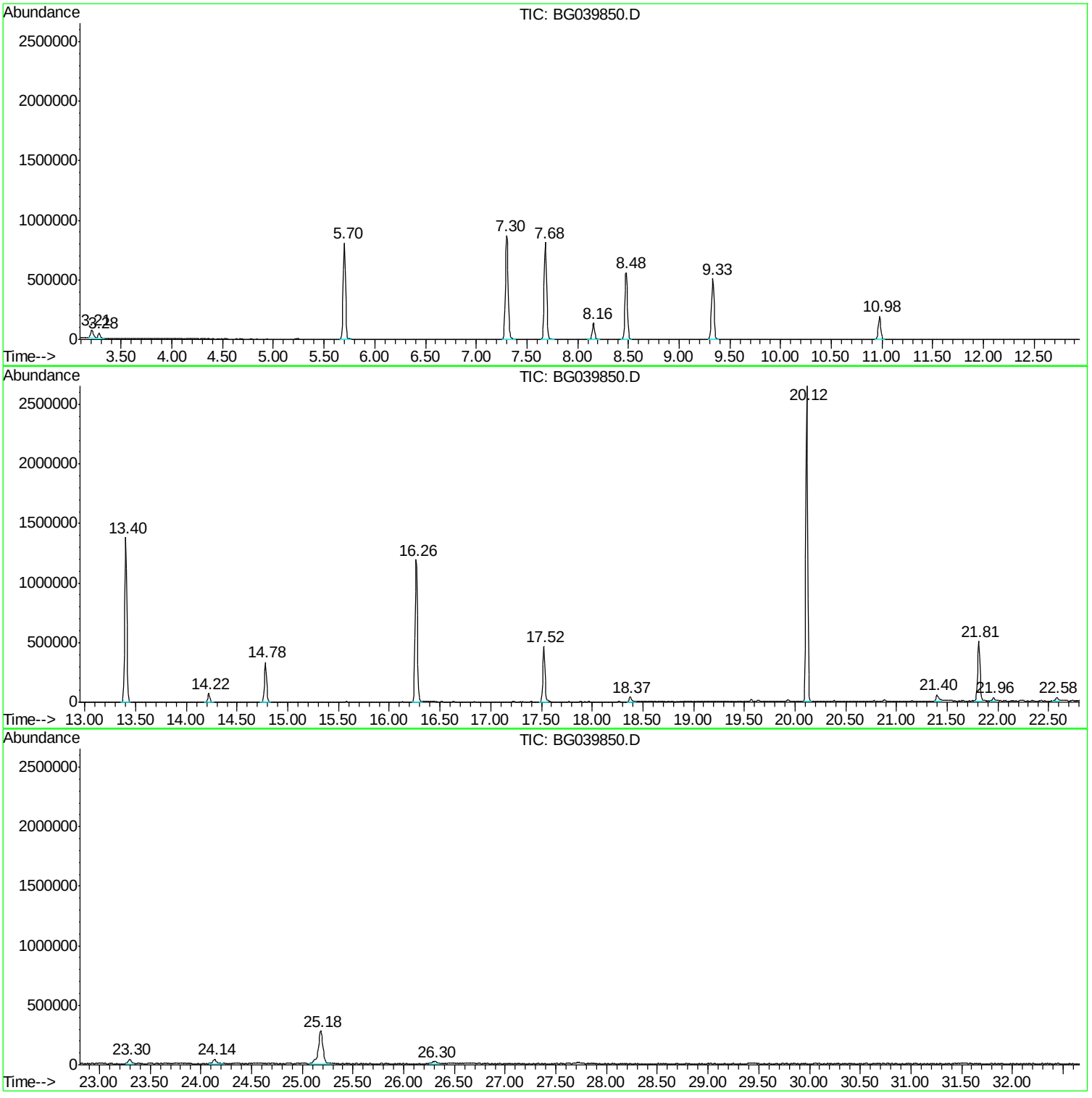
Sum of corrected areas: 18007252

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031119\
Data File : BG039850.D
Acq On : 11 Mar 2019 20:28
Operator : JU/SJ
Sample : K1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MR-MH-11-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031119\
Data File : BG039850.D
Acq On : 11 Mar 2019 20:28
Operator : JU/SJ
Sample : K1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MR-MH-11-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

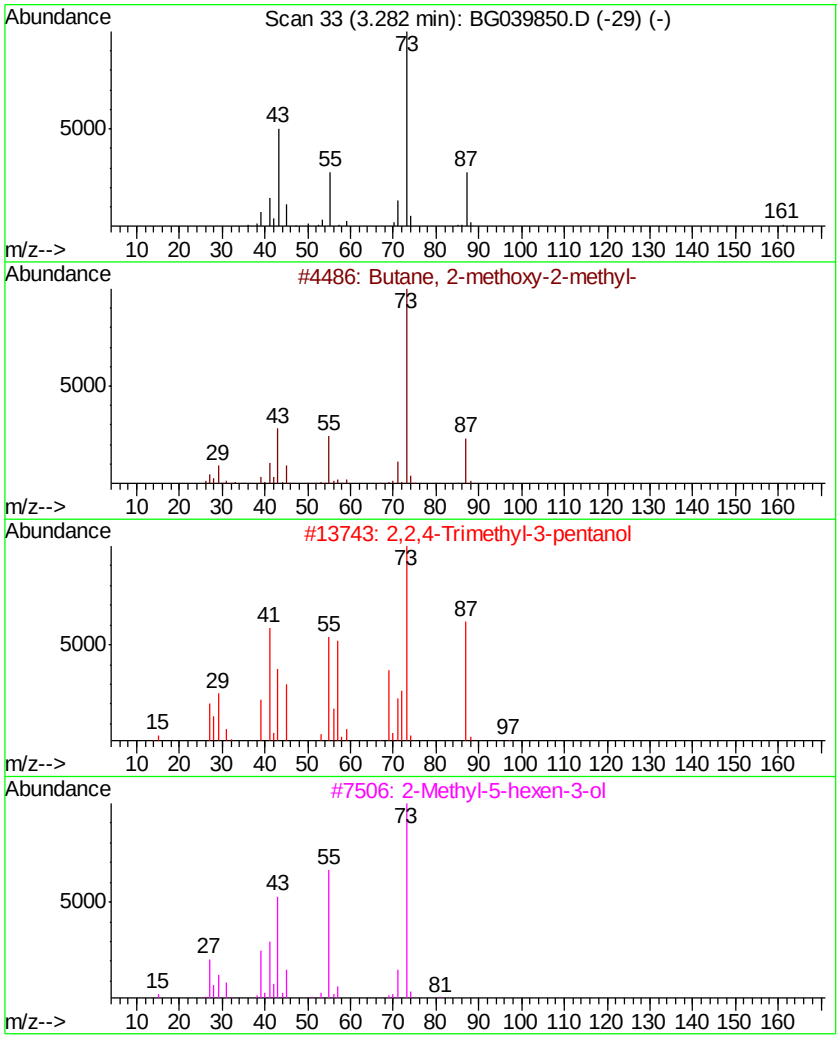
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

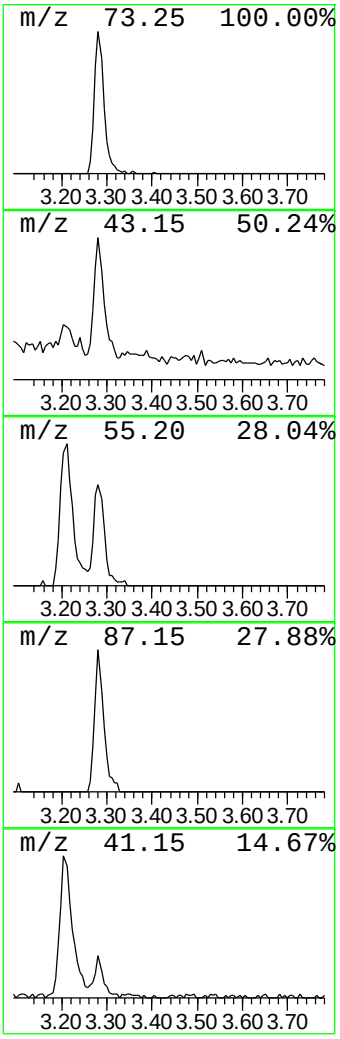
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	5.93 ng	71218	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	25
5	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031119\
Data File : BG039850.D
Acq On : 11 Mar 2019 20:28
Operator : JU/SJ
Sample : K1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MR-MH-11-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

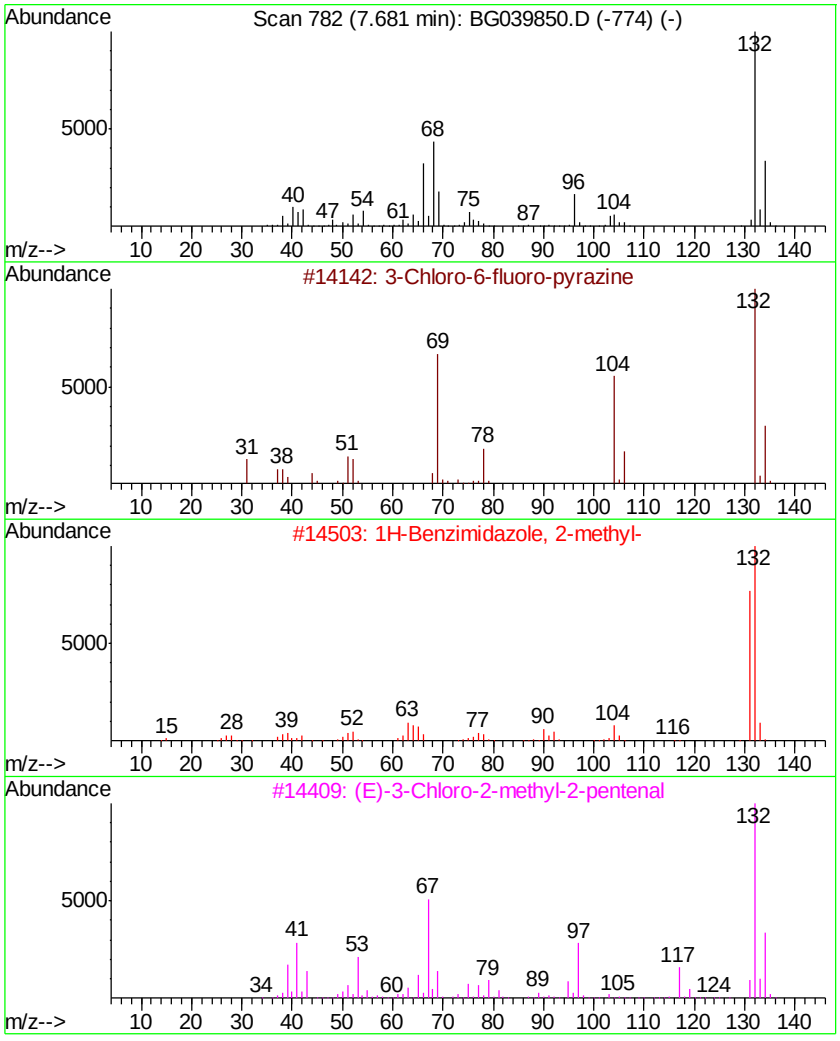
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

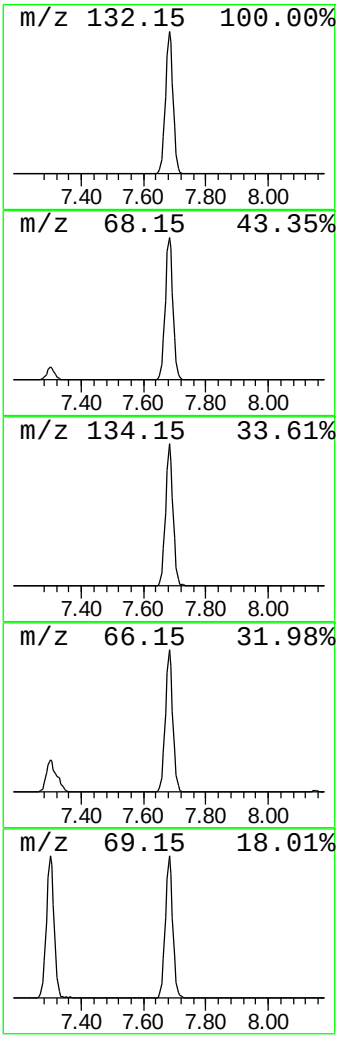
****

Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	115.87 ng	1392360	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031119\
Data File : BG039850.D
Acq On : 11 Mar 2019 20:28
Operator : JU/SJ
Sample : K1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MR-MH-11-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

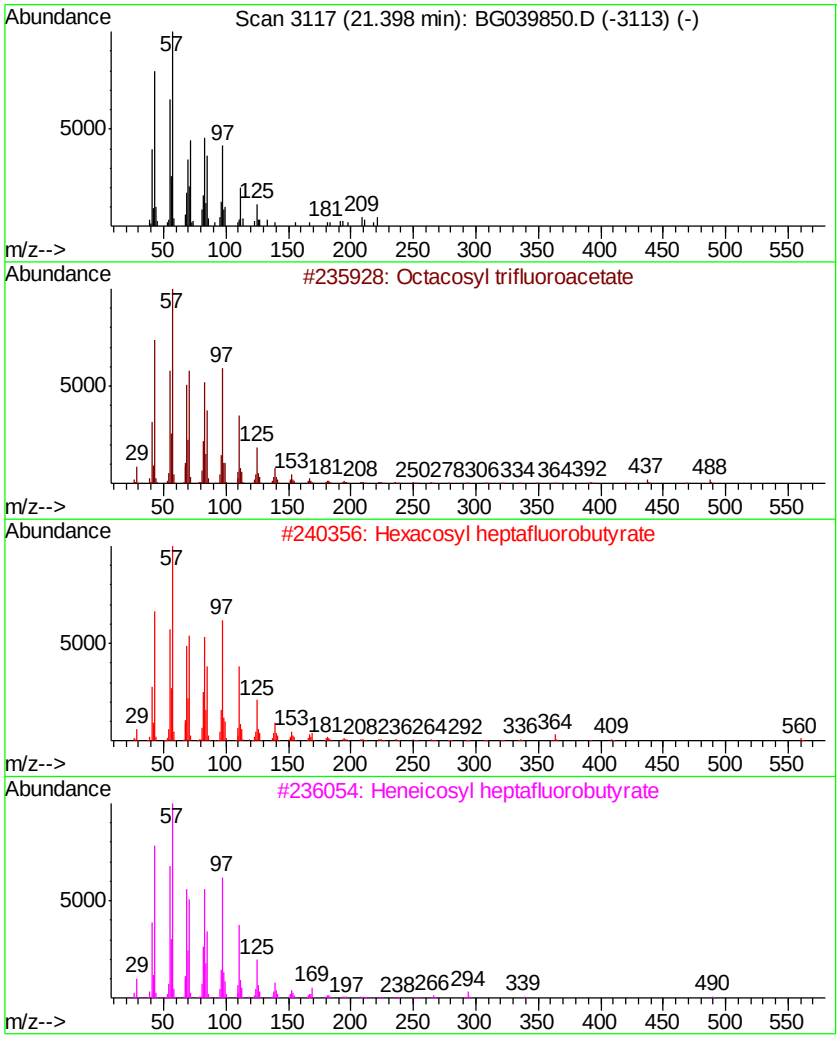
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

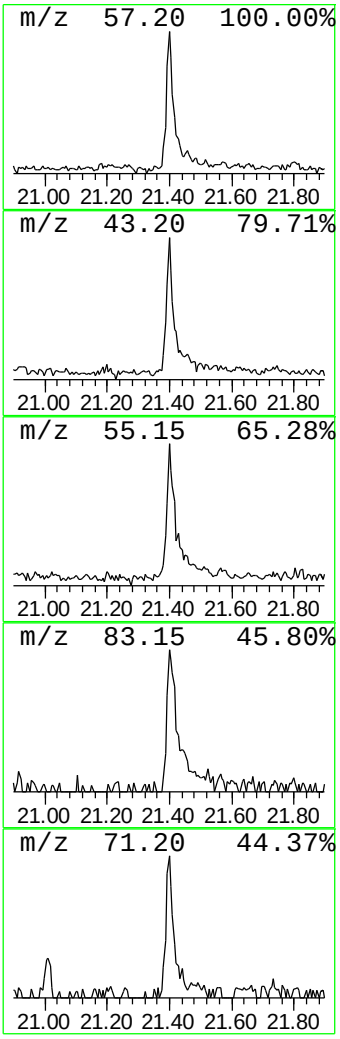
****

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.28 ng	99985	Chrysene-d12	21.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90
5	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG031119\
Data File : BG039850.D
Acq On : 11 Mar 2019 20:28
Operator : JU/SJ
Sample : K1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MR-MH-11-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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
Butane, 2-methoxy...	3.28	5.9	ng	71218	1	8.16	240331	20.0
unknown7.68	7.68	115.9	ng	1392360	1	8.16	240331	20.0
Octacosyl trifluo...	21.40	2.3	ng	99985	5	21.81	875922	20.0