LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082418\
Data File : BG036407.D
Acq On : 24 Aug 2018 10:31
Operator : JU/SJ
Sample : J4568-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 081718-SIDI-E-U-S

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-BG082318.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	5.167	315	320	329	rVB	30367	47447	1.07%	0.250%
2	5.632	392	399	409	rVB	381416	580335	13.07%	3.062%
3	7.218	661	669	677	rBV	241735	409974	9.23%	2.163%
4	7.594	726	733	741	rBV	627152	1058358	23.84%	5.585%
5	8.064	805	813	821	rBV	181467	309037	6.96%	1.631%
6	8.387	859	868	877	rBV	845707	1487450	33.50%	7.849%
7	9.227	1001	1011	1020	rBV	730183	1286716	28.98%	6.790%
8	10.873	1284	1291	1299	rBV	249899	442274	9.96%	2.334%
9	13.317	1699	1707	1715	rBV	2014886	3095295	69.71%	16.333%
10	14.139	1842	1847	1852	rBV	40794	56938	1.28%	0.300%
11	14.692	1934	1941	1951	rVB2	418529	660615	14.88%	3.486%
12	15.984	2157	2161	2166	rVB	63851	78368	1.76%	0.414%
13	16.172	2186	2193	2205	rBV	1055475	1583167	35.65%	8.354%
14	17.435	2401	2408	2414	rBV	540506	861002	19.39%	4.543%
15	18.323	2555	2559	2568	rBV3	53533	83435	1.88%	0.440%
16	20.044	2845	2852	2858	rBV	3279579	4440244	100.00%	23.430%
17	21.354	3070	3075	3089	rBV2	58468	149068	3.36%	0.787%
18	21.695	3126	3133	3145	rBV	644951	1107264	24.94%	5.843%
19	24.915	3670	3681	3691	rBV2	383194	1058292	23.83%	5.584%
20	25.015	3693	3698	3704	rVB3	20359	45396	1.02%	0.240%
21	26.155	3887	3892	3903	rVB4	21928	55881	1.26%	0.295%
22	27.529	4120	4126	4137	rVB7	17805	54881	1.24%	0.290%

Sum of corrected areas: 18951437

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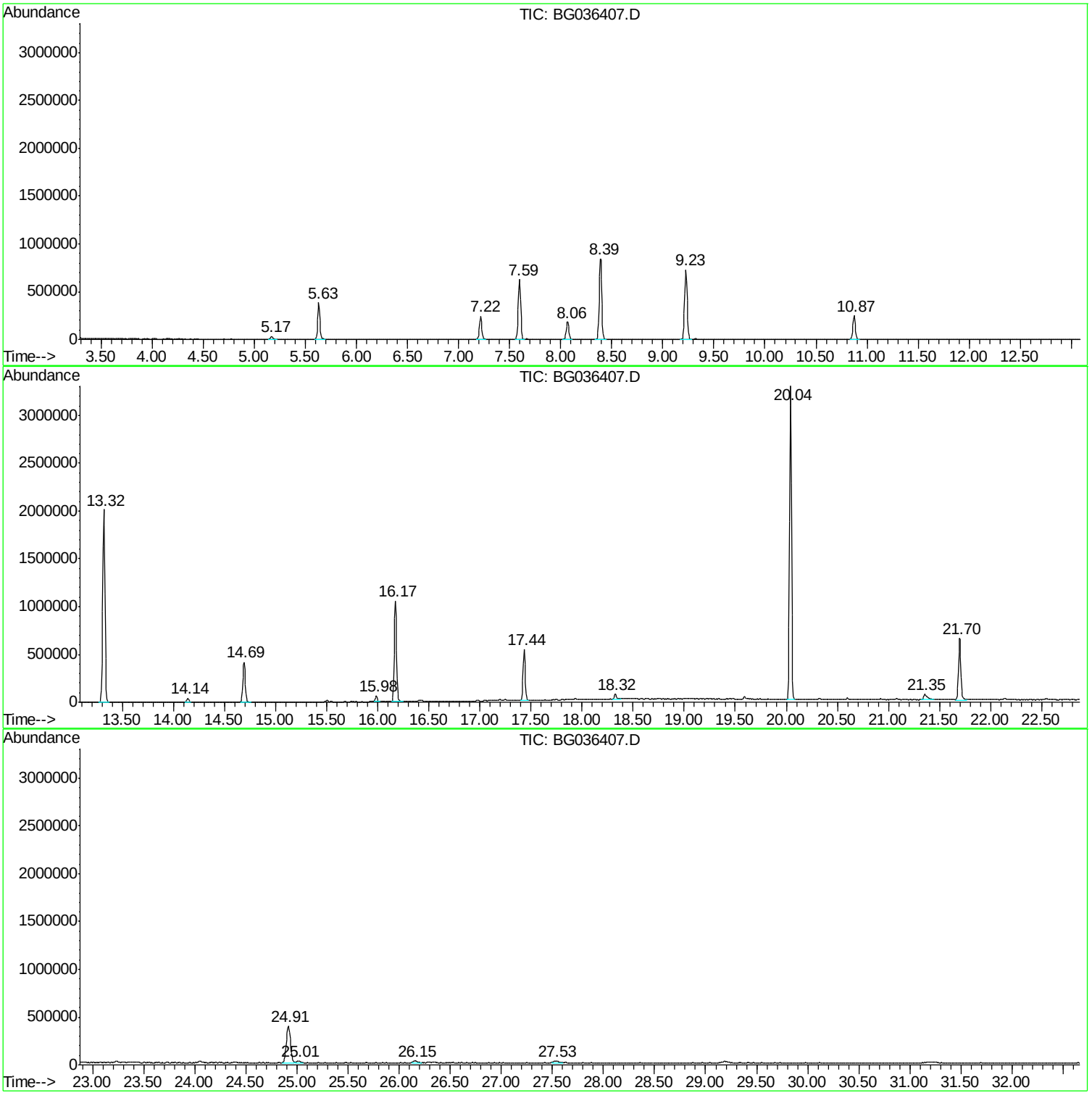
BNA_G
ClientSampleId :
081718-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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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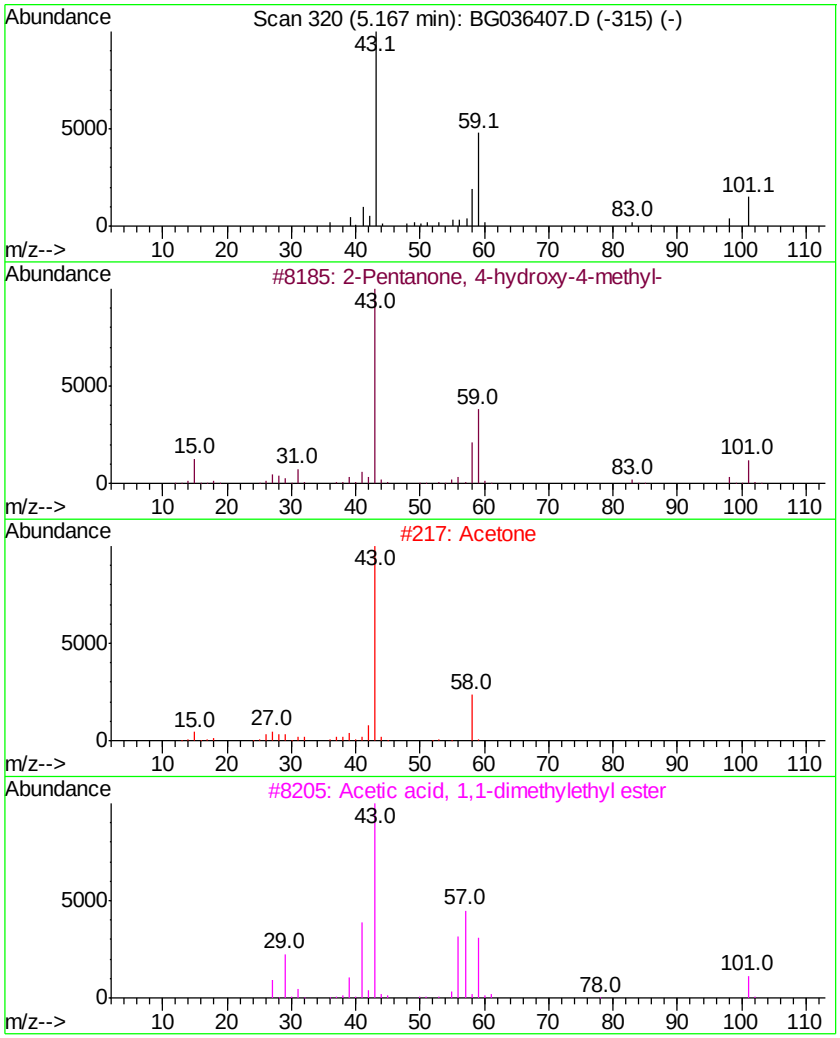
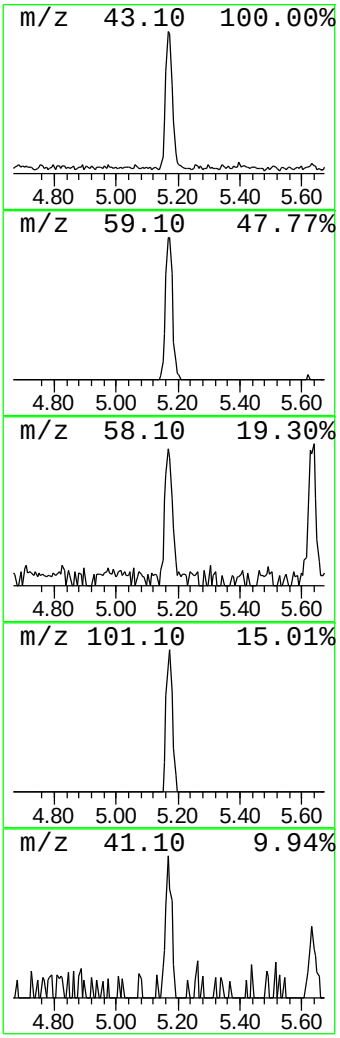
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.07 ng	47447	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	78
2	Acetone	58	C3H6O	000067-64-1	22
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	7
5	Diacetamide	101	C4H7NO2	000625-77-4	7





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082418\
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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 081718-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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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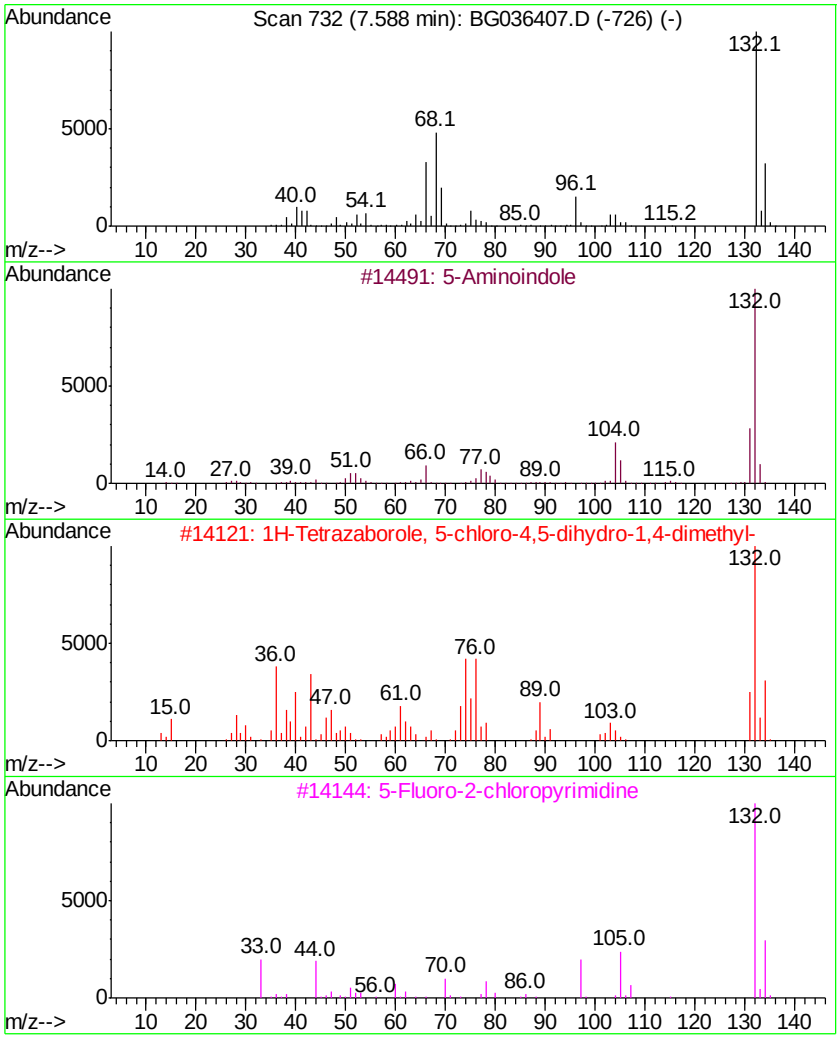
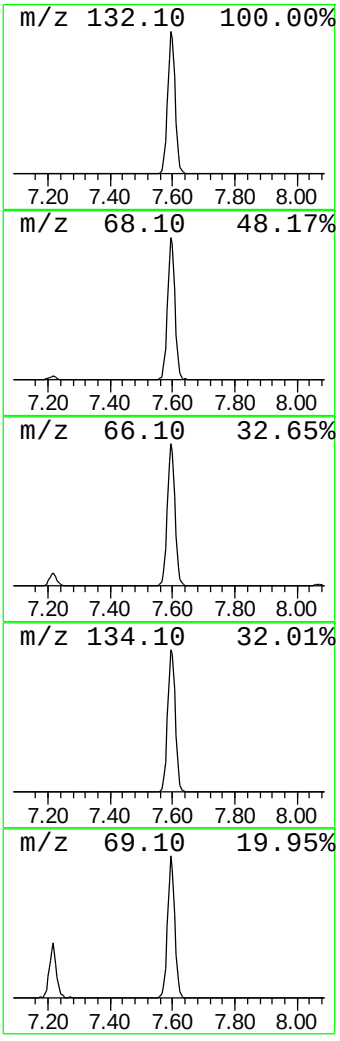
Peak Number 2 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	68.49 ng	1058360	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Instrument : BNA_G
ClientSampleId : 081718-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
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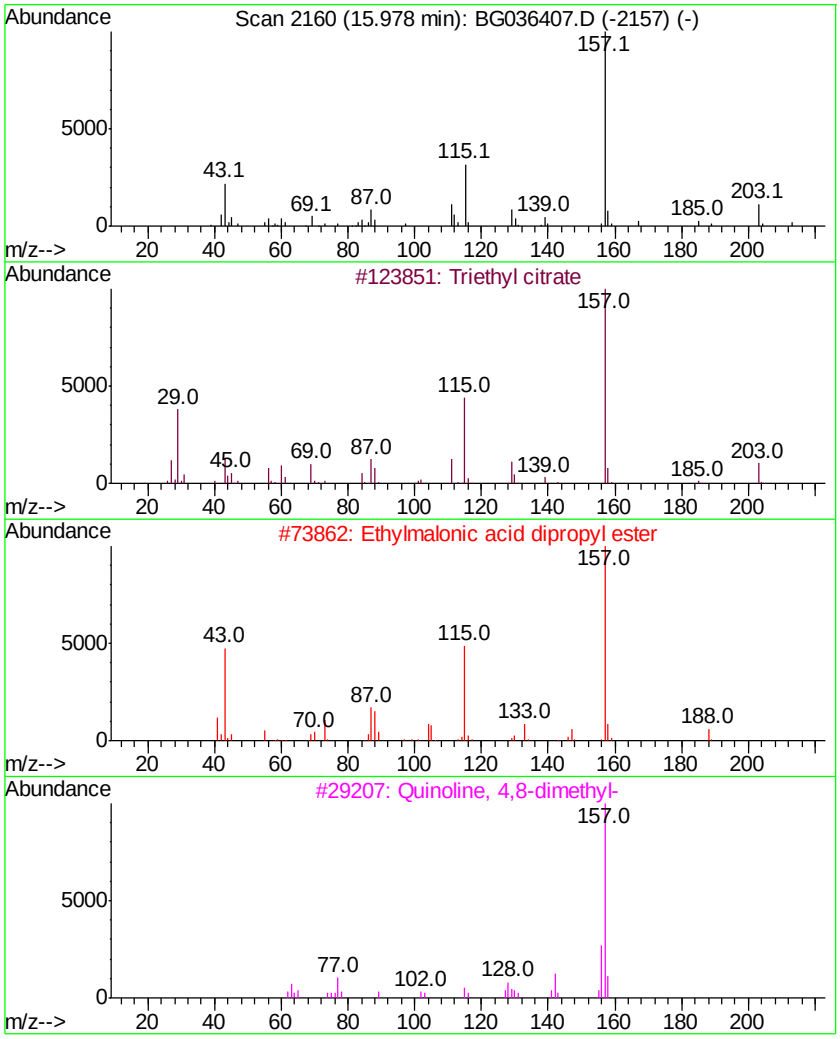
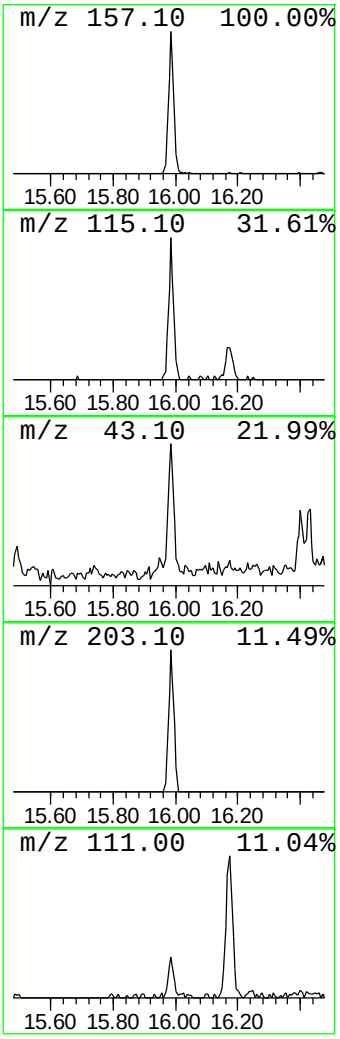
Peak Number 4 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.37 ng	78368	Acenaphthene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	83
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
3	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40
4	Hexanedioic acid, 3-ethyl-, bis(...	286	C16H30O4	057983-54-7	39
5	Adipic acid, isobutyl 3-(2-metho...	358	C20H38O5	1000324-28-7	36





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Misc :
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Instrument : BNA_G
ClientSampleId : 081718-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
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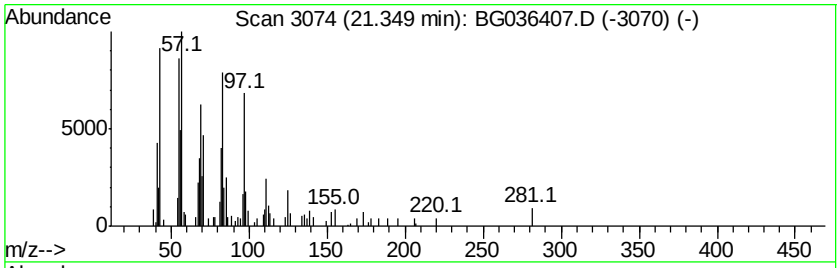
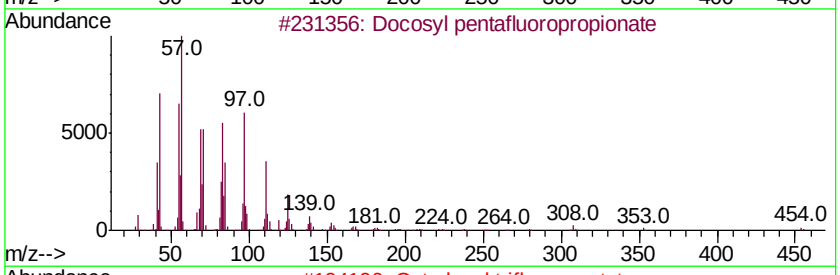
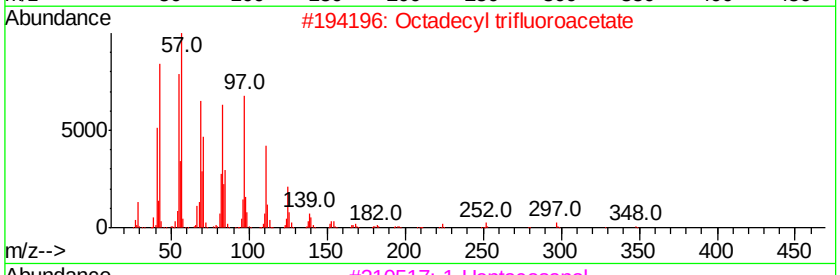
Peak Number 5 Docosyl pentafluoropropionate Concentration Rank 4

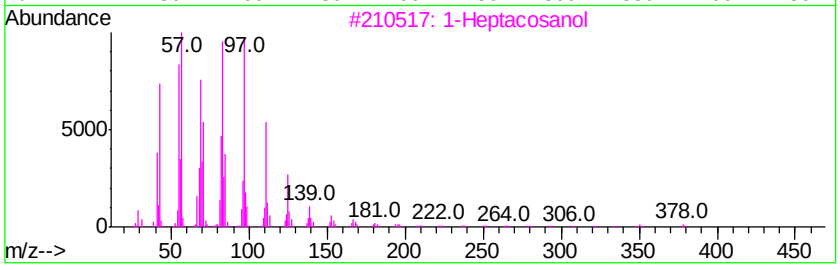
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	2.69 ng	149068	Chrysene-d12	21.70

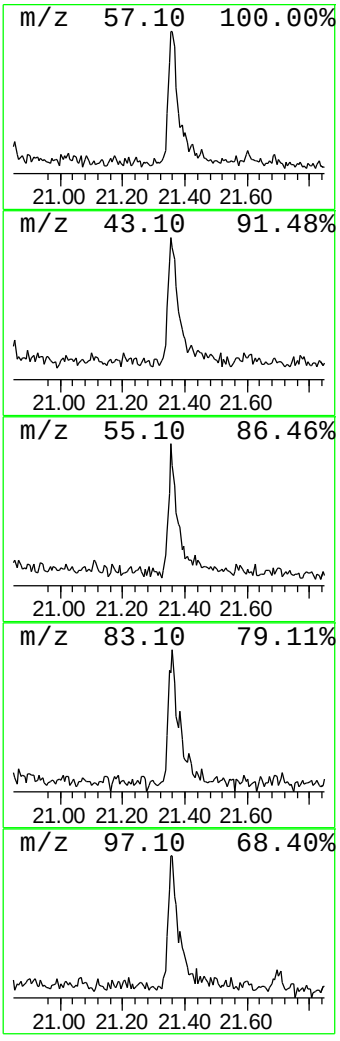
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91











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
2-Pentanone, 4-hy...	5.17	3.1	ng	47447	1	8.06	309037	20.0
unknown7.59	7.59	68.5	ng	1058360	1	8.06	309037	20.0
Triethyl citrate	15.98	2.4	ng	78368	3	14.69	660615	20.0
Docosyl pentafluo...	21.35	2.7	ng	149068	5	21.70	1107260	20.0