LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040418\
Data File : BG033567.D
Acq On : 4 Apr 2018 19:36
Operator : SJ/JU
Sample : J2177-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 032818-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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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	3.482	27	33	43	rBV	137666	274089	7.00%	1.810%
2	3.571	43	48	60	rVB	118867	192211	4.91%	1.270%
3	5.774	418	423	429	rBV	30309	50003	1.28%	0.330%
4	6.291	503	511	532	rBV	136232	329438	8.41%	2.176%
5	7.977	791	798	815	rBV	78975	237602	6.06%	1.569%
6	8.377	859	866	884	rBV	299384	686727	17.53%	4.536%
7	8.864	943	949	968	rBV2	75541	199226	5.08%	1.316%
8	9.193	997	1005	1022	rBV	446878	933808	23.83%	6.168%
9	10.063	1146	1153	1180	rBV	382882	894900	22.84%	5.911%
10	11.743	1430	1439	1452	rBV	128893	298613	7.62%	1.972%
11	14.105	1834	1841	1862	rBV	1352944	2336851	59.64%	15.435%
12	14.899	1969	1976	1982	rBV2	26814	46344	1.18%	0.306%
13	15.480	2069	2075	2088	rBV2	311507	546520	13.95%	3.610%
14	16.955	2319	2326	2340	rBV	818475	1425216	36.37%	9.414%
15	17.096	2347	2350	2359	rVB3	23995	43349	1.11%	0.286%
16	18.212	2533	2540	2553	rBV	440650	784864	20.03%	5.184%
17	19.005	2671	2675	2684	rBV3	28372	52978	1.35%	0.350%
18	20.733	2962	2969	2983	rBV	2738589	3918200	100.00%	25.880%
19	22.072	3191	3197	3202	rBV3	70823	139101	3.55%	0.919%
20	22.560	3271	3280	3295	rBV	436637	894557	22.83%	5.909%
21	26.320	3905	3920	3938	rBV3	223236	855300	21.83%	5.649%

Sum of corrected areas: 15139897

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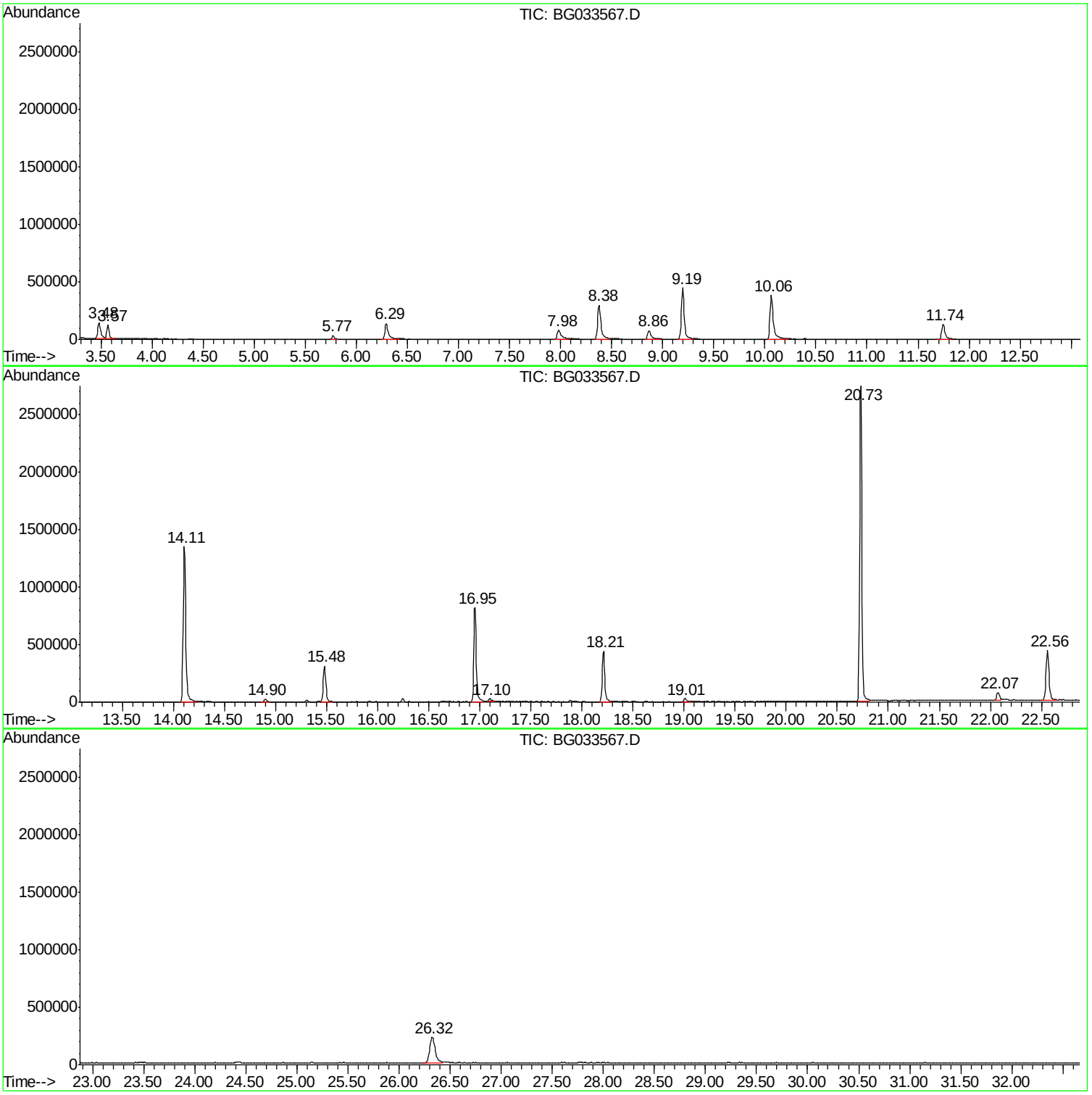
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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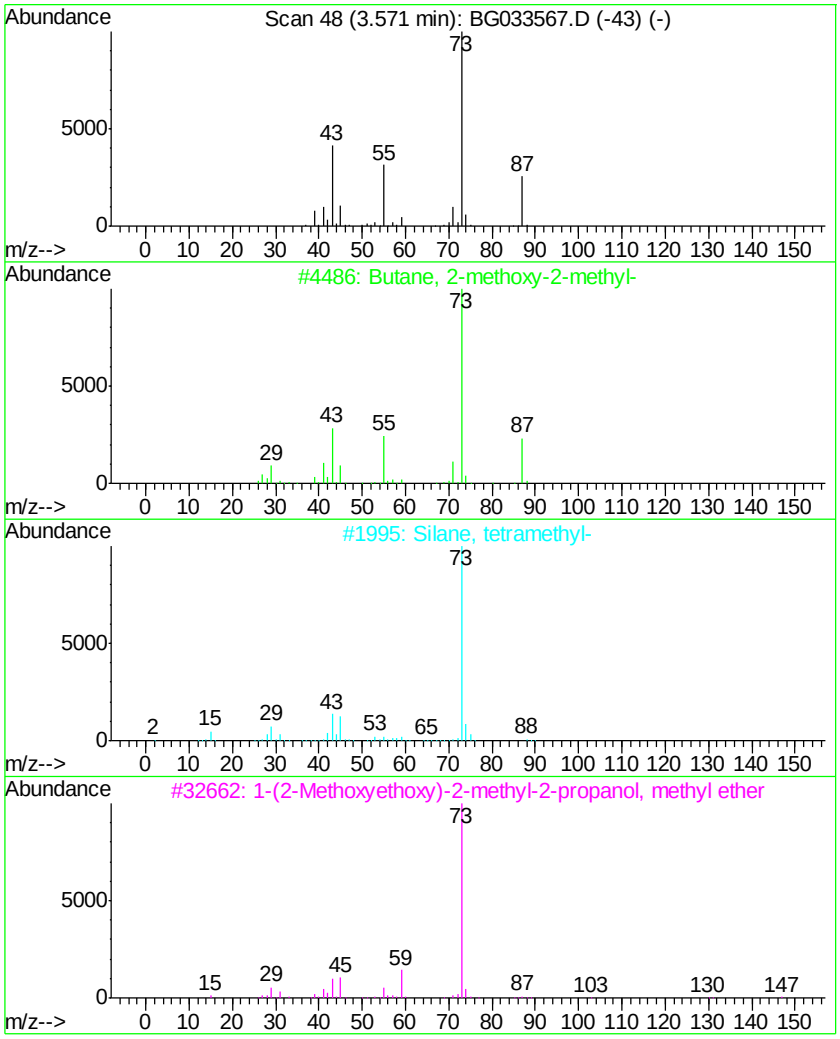
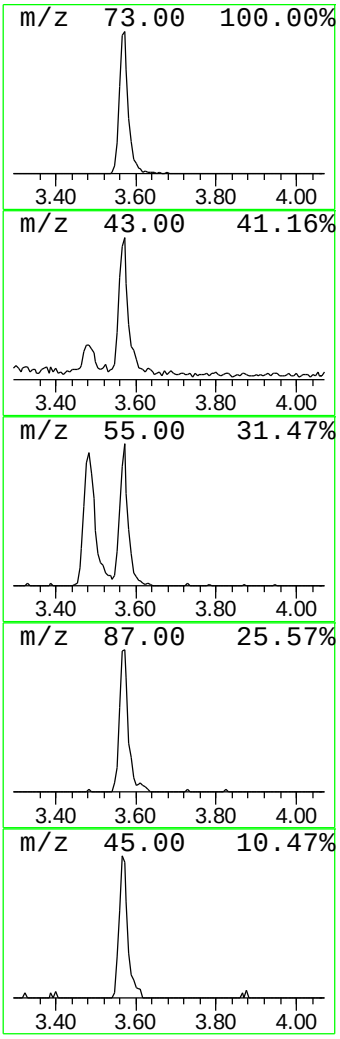
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	19.30 ng	192211	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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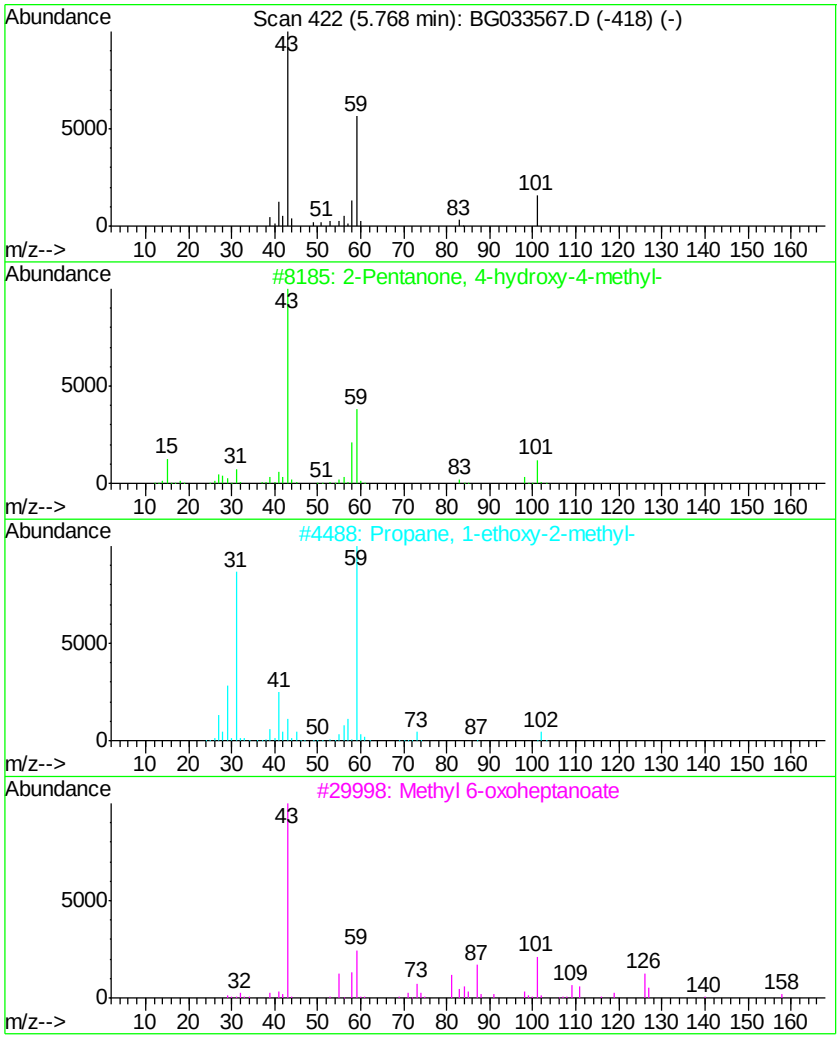
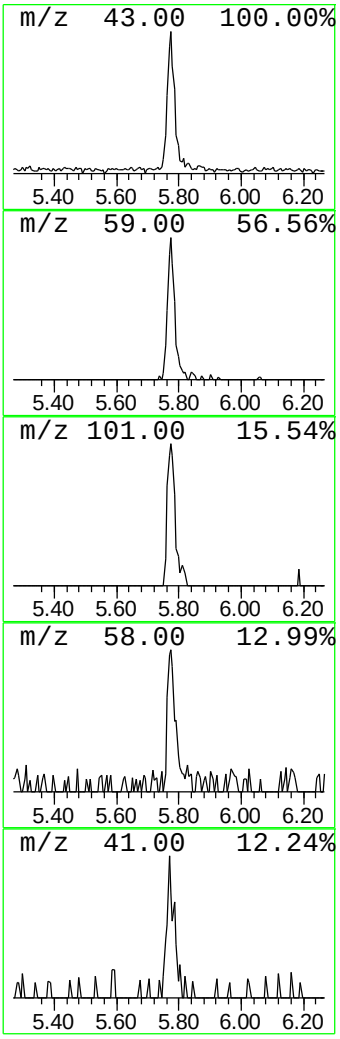
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	5.02 ng	50003	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12
3	Methyl 6-oxoheptanoate	158	C8H14O3	002046-21-1	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_G
ClientSampleId : 032818-SIDI-E-U-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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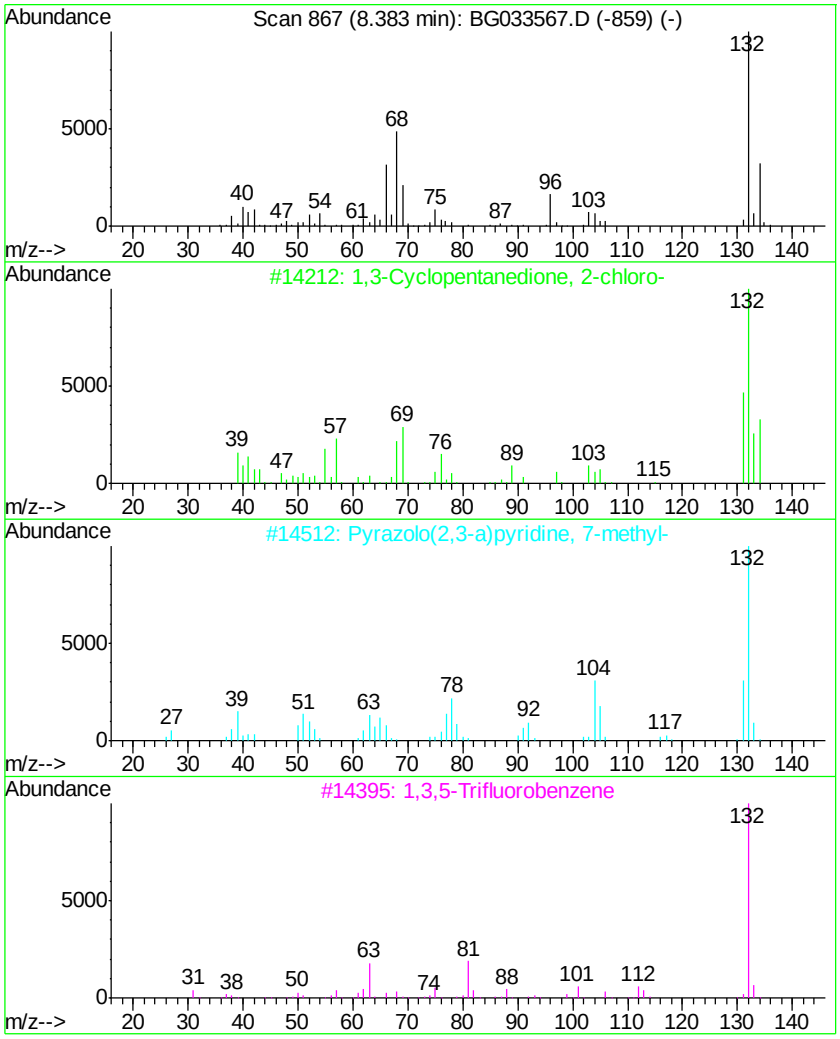
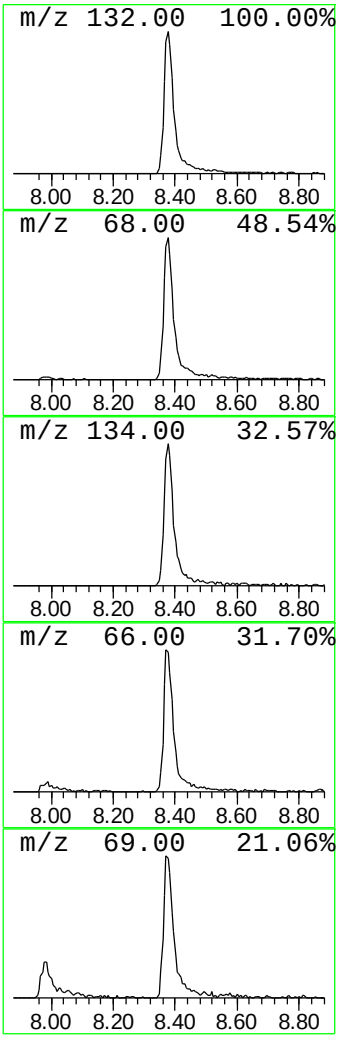
Peak Number 4 unknown8.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	68.94 ng	686727	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
2	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Library Search Compound Report

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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 032818-SIDI-E-U-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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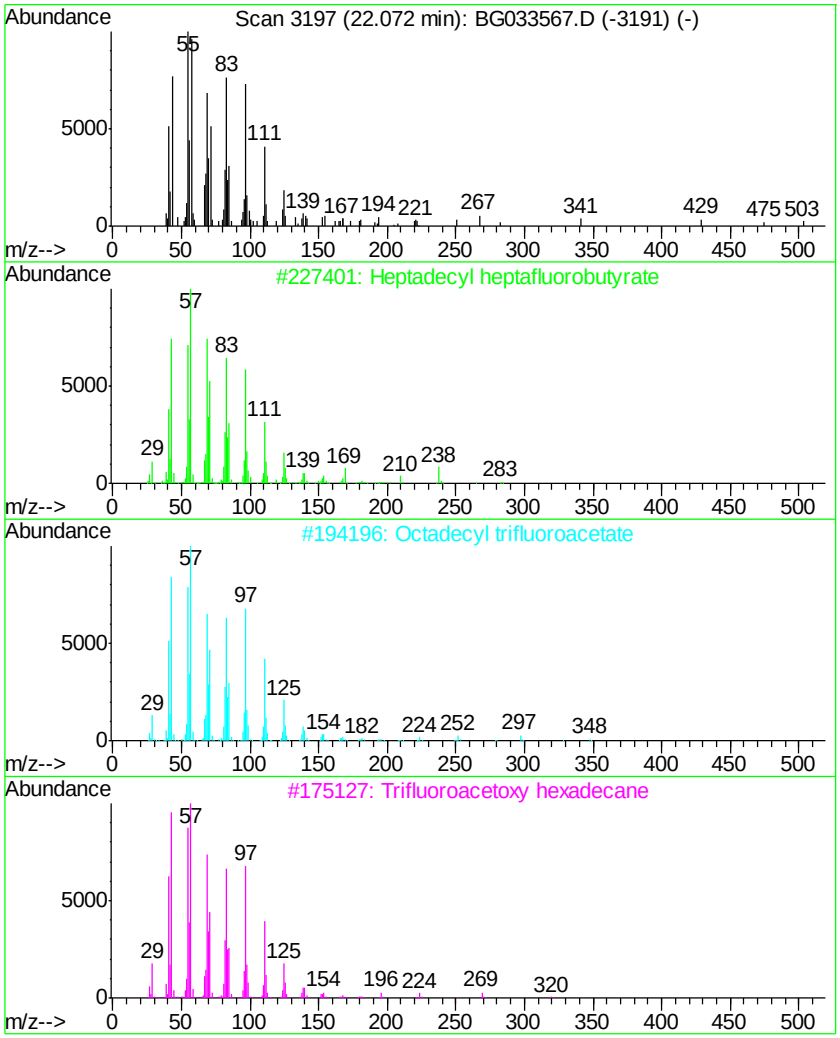
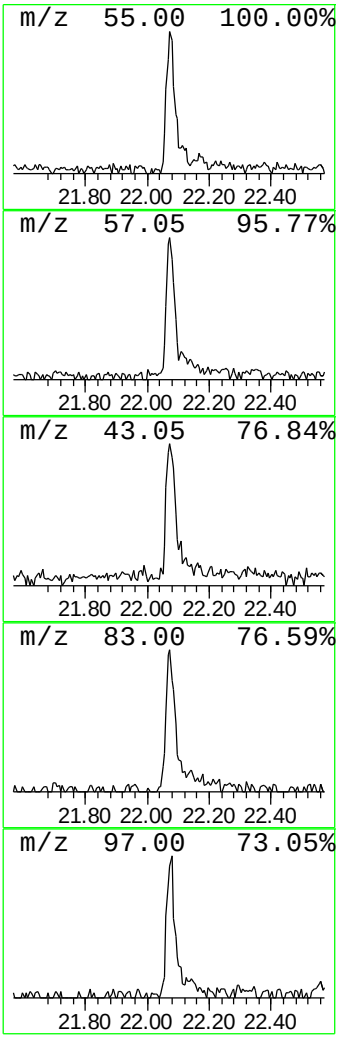
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	3.11 ng	139101	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	19.3	ng	192211	1	8.86	199226	20.0
2-Pentanone, 4-hy...	5.77	5.0	ng	50003	1	8.86	199226	20.0
unknown8.38	8.38	68.9	ng	686727	1	8.86	199226	20.0
Heptadecyl heptaf...	22.07	3.1	ng	139101	5	22.56	894557	20.0