LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010419\
Data File : BG038942.D
Acq On : 4 Jan 2019 23:04
Operator : JU/SJ
Sample : K1029-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B1_123118

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-BG121218.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	3.167	9	13	22	rVB	37632	59453	2.64%	0.624%
2	5.130	341	347	355	rBV	12833	22650	1.00%	0.238%
3	5.600	420	427	437	rBV	174167	297339	13.18%	3.120%
4	7.204	693	700	712	rBV	115247	214960	9.53%	2.256%
5	7.574	756	763	773	rBV	349644	623958	27.66%	6.547%
6	8.044	836	843	850	rBV	88470	148516	6.58%	1.558%
7	8.367	890	898	907	rVB	325983	583294	25.86%	6.121%
8	9.225	1036	1044	1059	rBV	279491	524746	23.26%	5.506%
9	10.864	1315	1323	1332	rBV	114934	212977	9.44%	2.235%
10	13.302	1731	1738	1749	rBV	882237	1375693	60.98%	14.435%
11	14.131	1871	1879	1885	rBV	25673	43216	1.92%	0.453%
12	14.683	1965	1973	1984	rBV2	200488	342314	15.17%	3.592%
13	16.175	2220	2227	2242	rBV3	696221	1176380	52.15%	12.344%
14	17.433	2434	2441	2449	rBV2	286080	438355	19.43%	4.600%
15	20.036	2878	2884	2895	rBV	1673035	2255952	100.00%	23.672%
16	21.305	3096	3100	3109	rBV3	26059	51361	2.28%	0.539%
17	21.710	3162	3169	3181	rBV	269736	482633	21.39%	5.064%
18	22.456	3291	3296	3304	rBV5	13776	29394	1.30%	0.308%
19	23.156	3410	3415	3420	rVB2	17815	34460	1.53%	0.362%
20	23.349	3443	3448	3456	rVB3	19795	40218	1.78%	0.422%
21	23.960	3548	3552	3562	rVB5	20338	48954	2.17%	0.514%
22	24.924	3708	3716	3720	rBV2	15823	39516	1.75%	0.415%
23	25.006	3720	3730	3744	rVB2	151349	449746	19.94%	4.719%
24	26.058	3902	3909	3919	rVB6	12060	33995	1.51%	0.357%

Sum of corrected areas: 9530080

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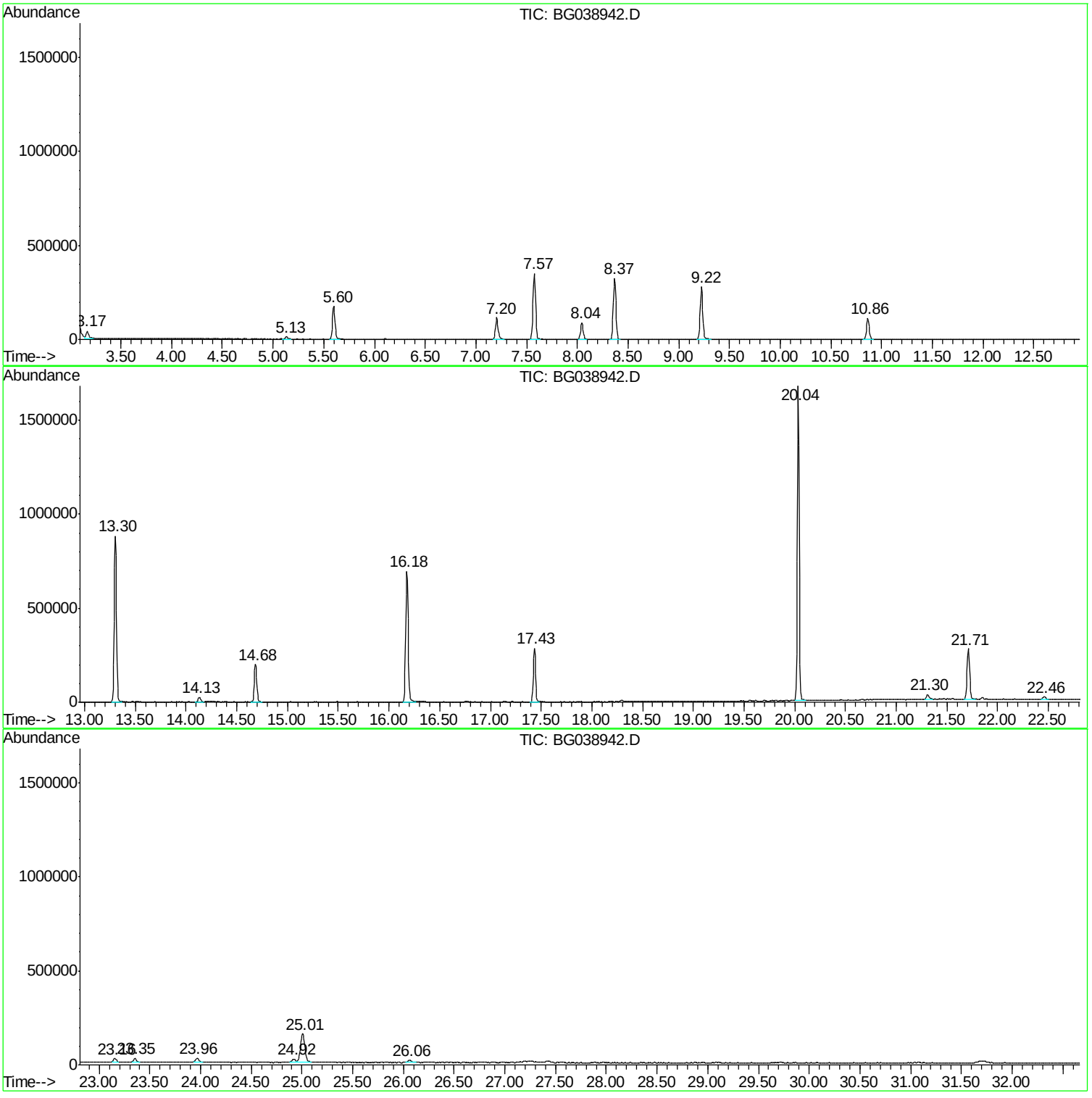
ClientSampleId : B1_123118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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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Data File : BG038942.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

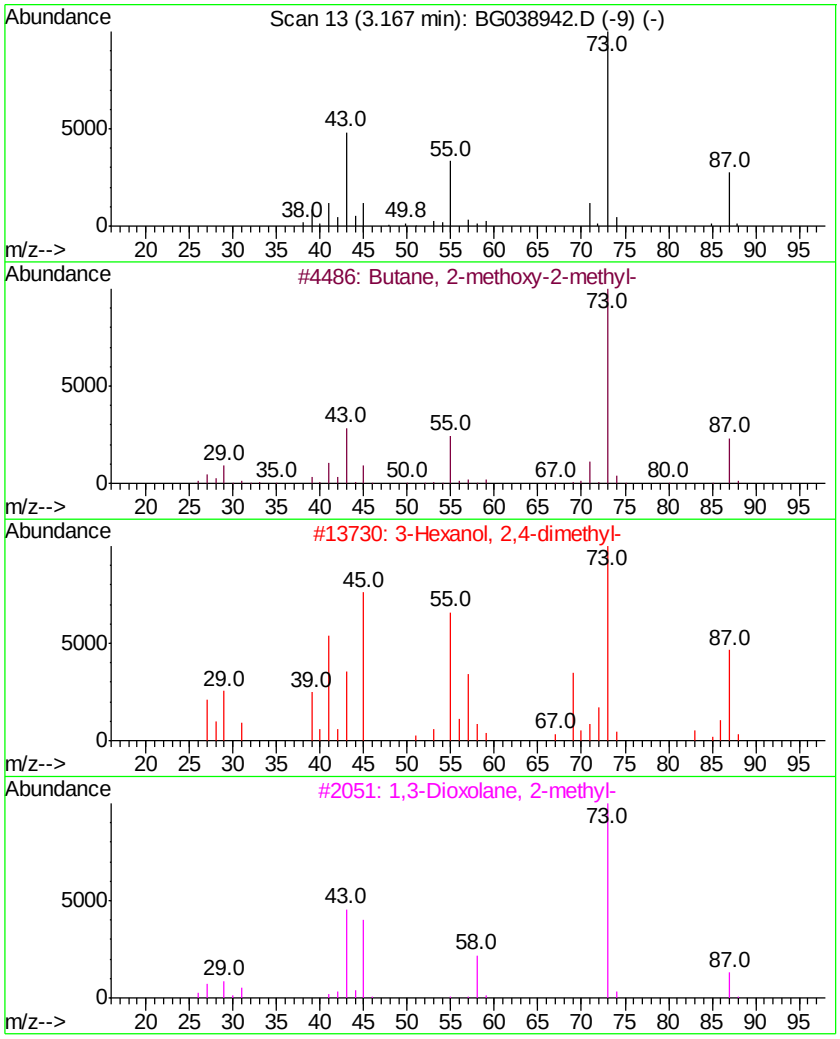
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

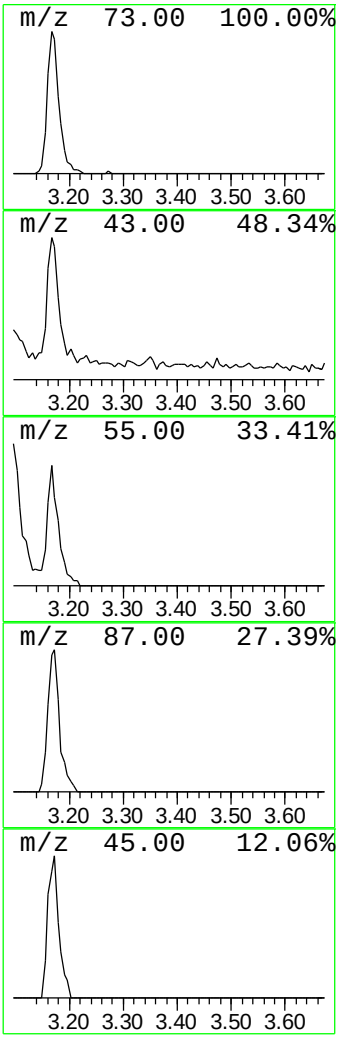
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	8.01 ng	59453	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	45
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	25
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Data File : BG038942.D
Acq On : 4 Jan 2019 23:04
Operator : JU/SJ
Sample : K1029-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B1_123118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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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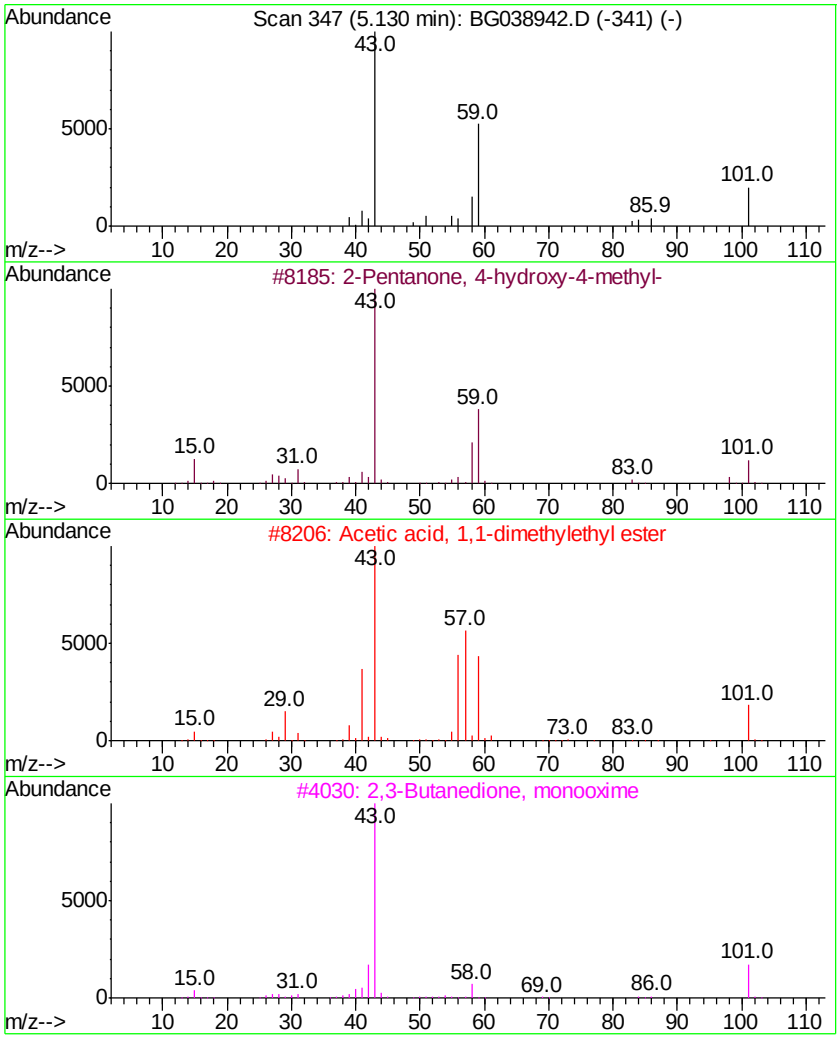
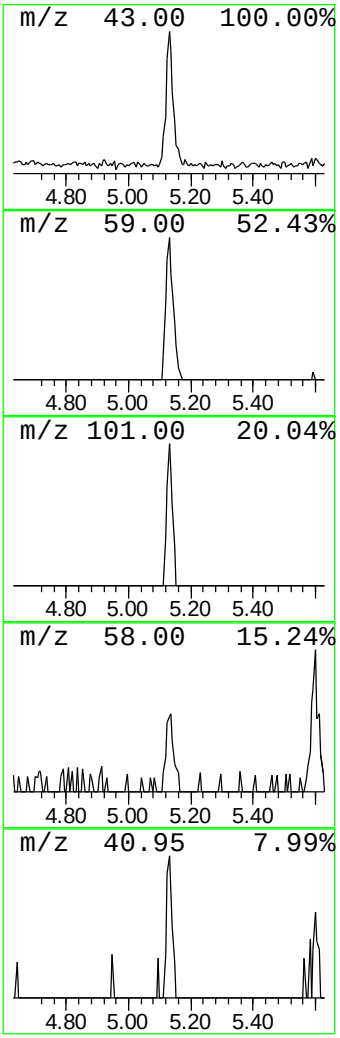
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.05 ng	22650	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5
5	Oxetane, 2,2-dimethyl-	86	C5H10O	006245-99-4	4





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010419\
Data File : BG038942.D
Acq On : 4 Jan 2019 23:04
Operator : JU/SJ
Sample : K1029-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B1_123118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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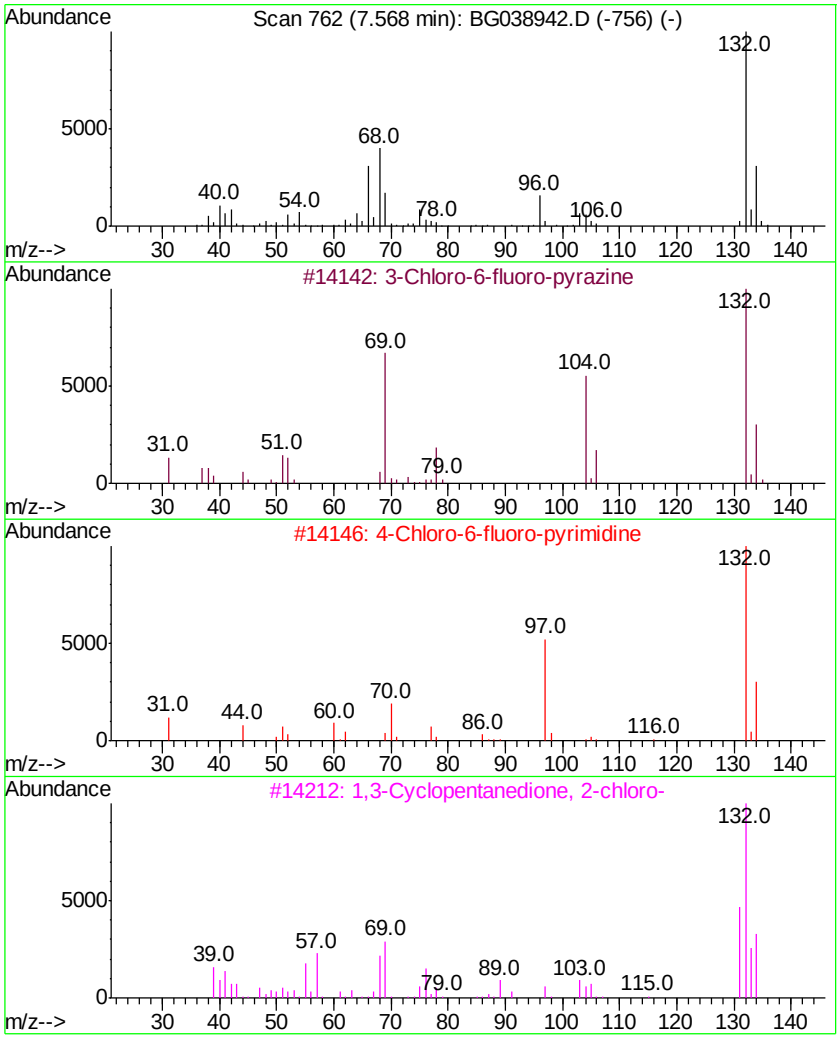
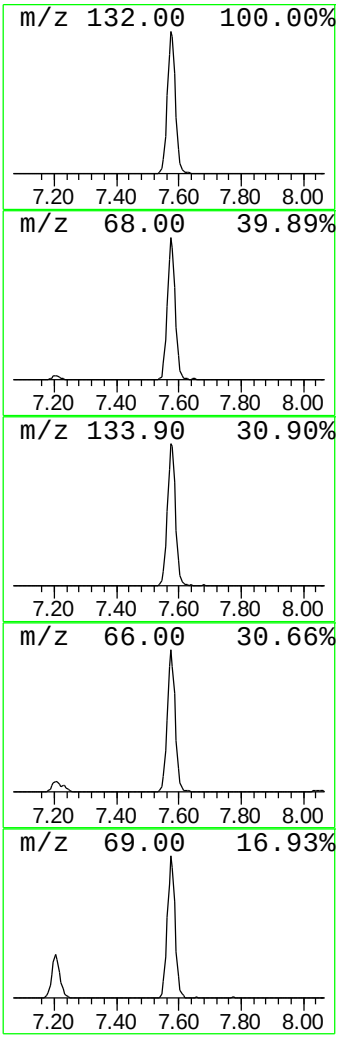
Peak Number 3 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	84.03 ng	623958	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B1_123118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
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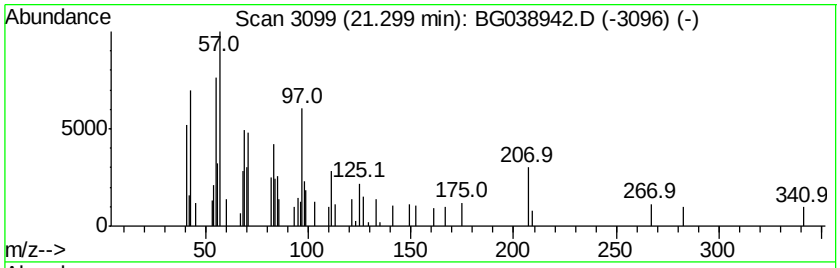
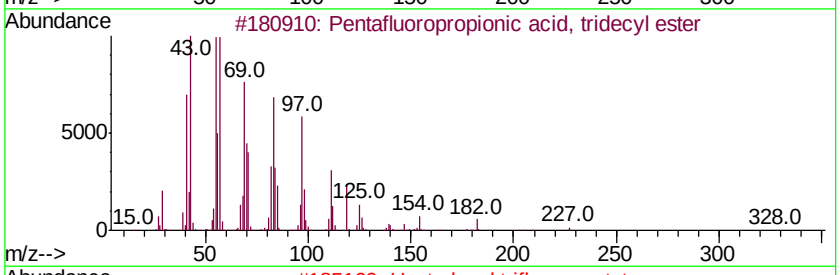
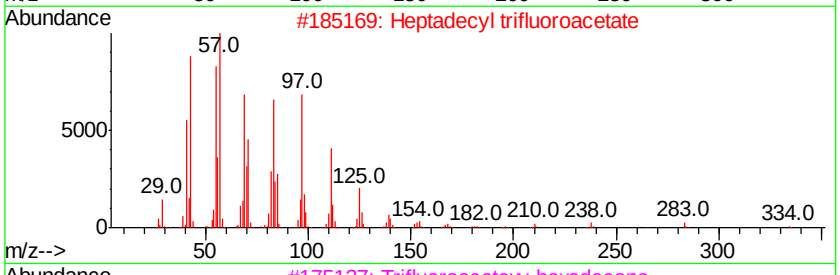
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 6

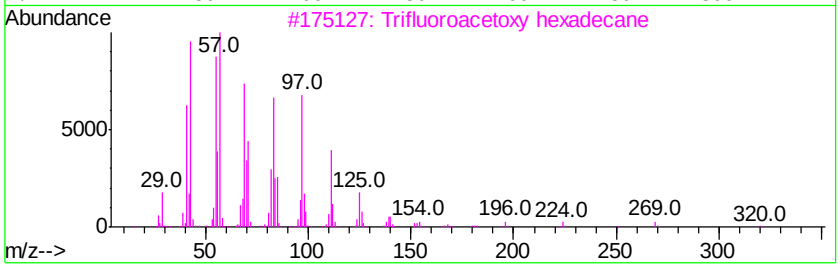
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	2.13 ng	51361	Chrysene-d12	21.71

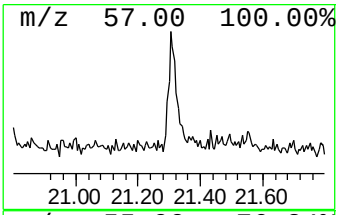
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	86
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	72
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	68
4	Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	64
5	1-Heneicosanol	312	C21H44O	015594-90-8	62

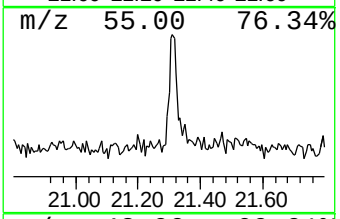


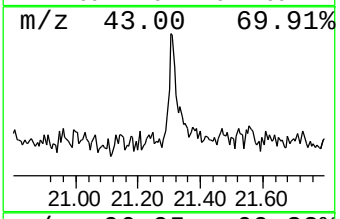


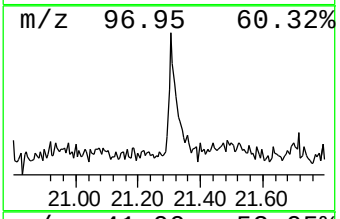


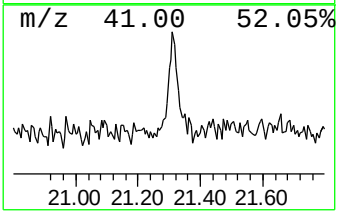












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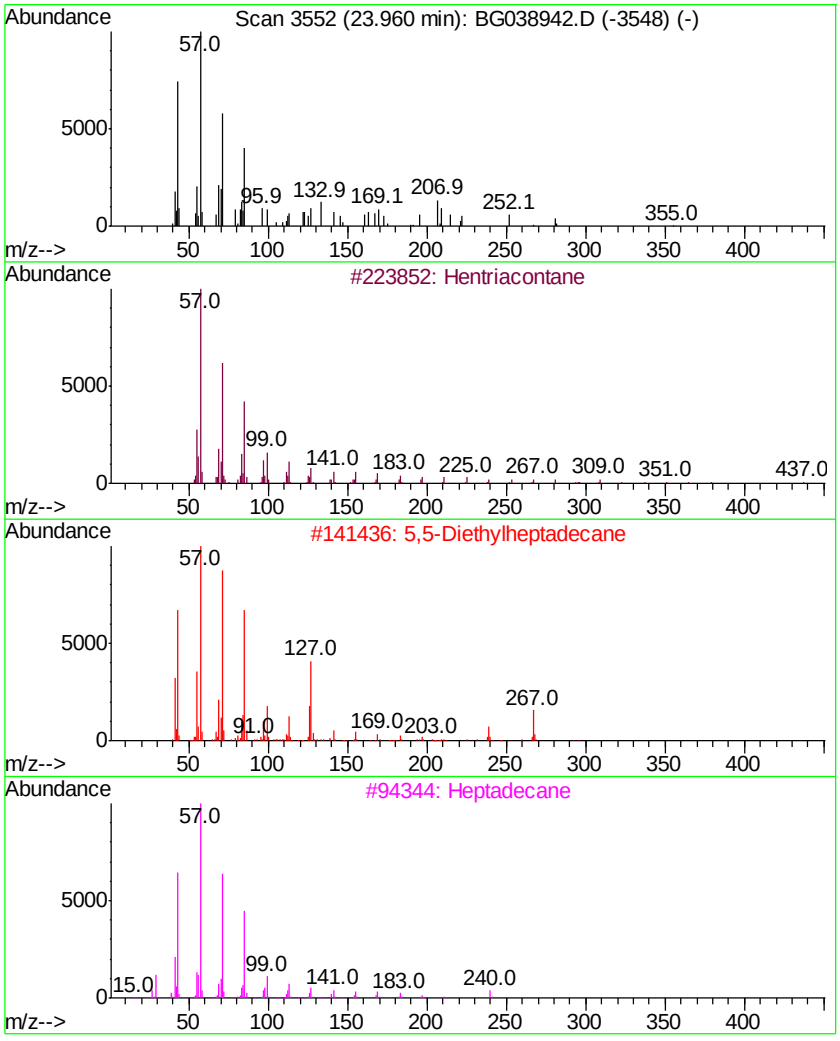
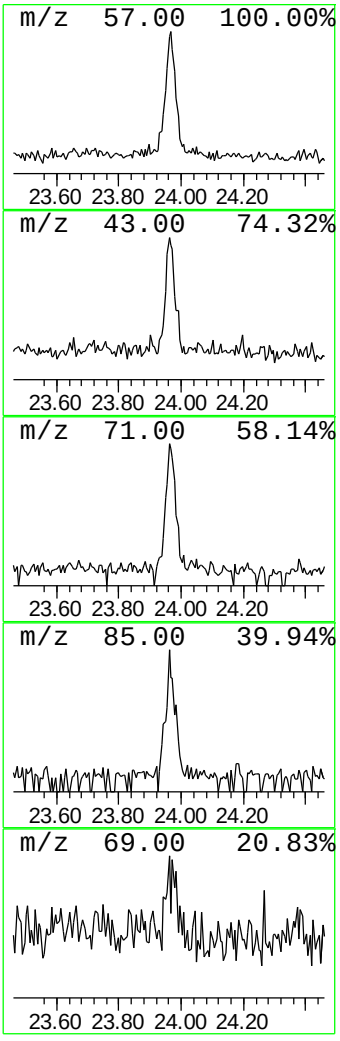
****

Peak Number 6 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.96	2.18 ng	48954	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	50
2	5,5-Diethylheptadecane	296	C21H44	1000360-41-7	47
3	Heptadecane	240	C17H36	000629-78-7	47
4	Tritetracontane	605	C43H88	007098-21-7	47
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	47





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.17	8.0	ng	59453	1	8.04	148516	20.0
2-Pentanone, 4-hy...	5.13	3.0	ng	22650	1	8.04	148516	20.0
unknown7.57	7.57	84.0	ng	623958	1	8.04	148516	20.0
Pentafluoropropio...	21.30	2.1	ng	51361	5	21.71	482633	20.0
Hentriacontane	23.96	2.2	ng	48954	6	25.01	449746	20.0