LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049192.D
Acq On : 6 Jul 2021 19:35
Operator : CG/JU
Sample : M2926-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-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-BG063021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049192.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.132	10	16	25	rBV2	45042	126296	6.37%	1.190%
2	3.214	25	30	36	rVB4	19546	39324	1.98%	0.371%
3	5.171	358	363	368	rBV2	17705	31131	1.57%	0.293%
4	5.641	435	443	457	rBV	529440	921023	46.42%	8.679%
5	7.239	708	715	727	rBV	555924	1018002	51.31%	9.593%
6	7.374	733	738	744	rVB3	14586	25174	1.27%	0.237%
7	7.680	784	790	798	rBV4	11806	27018	1.36%	0.255%
8	8.085	852	859	867	rBV	136222	238191	12.01%	2.245%
9	9.254	1050	1058	1068	rBV	365599	653808	32.96%	6.161%
10	10.905	1331	1339	1350	rVB	175201	326508	16.46%	3.077%
11	13.349	1748	1755	1764	rBV	911026	1445489	72.86%	13.621%
12	14.172	1889	1895	1901	rBV	107022	155470	7.84%	1.465%
13	14.730	1984	1990	1997	rVB	272666	433169	21.83%	4.082%
14	16.217	2236	2243	2260	rBV	676420	1161296	58.53%	10.943%
15	17.480	2451	2458	2467	rVB	325442	512033	25.81%	4.825%
16	18.355	2602	2607	2611	rBV4	27760	42123	2.12%	0.397%
17	19.219	2750	2754	2762	rBV6	9750	20072	1.01%	0.189%
18	19.524	2802	2806	2812	rVB2	20525	28566	1.44%	0.269%
19	20.083	2895	2901	2909	rBV	1541334	1983941	100.00%	18.695%
20	21.393	3119	3124	3136	rVB2	116250	245327	12.37%	2.312%
21	21.757	3180	3186	3193	rBV	321355	537304	27.08%	5.063%
22	21.904	3208	3211	3217	rVB7	12031	22405	1.13%	0.211%
23	23.485	3476	3480	3486	rVB6	15279	32154	1.62%	0.303%
24	25.065	3739	3749	3765	rVB3	184638	586153	29.54%	5.524%

Sum of corrected areas: 10611977

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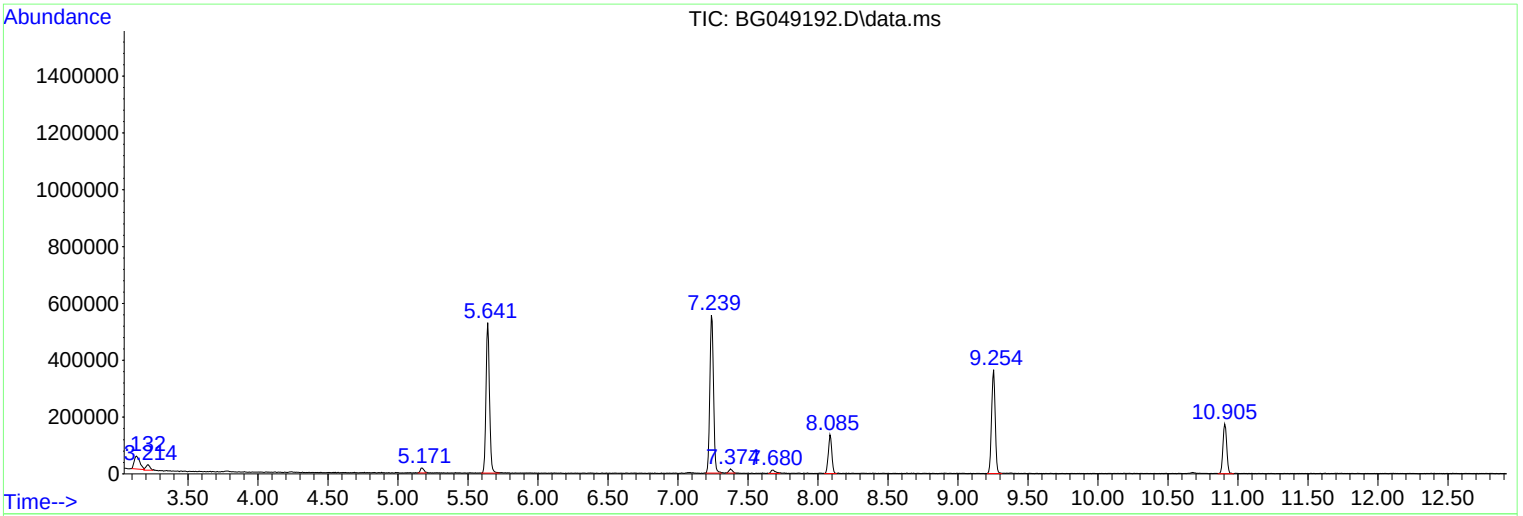
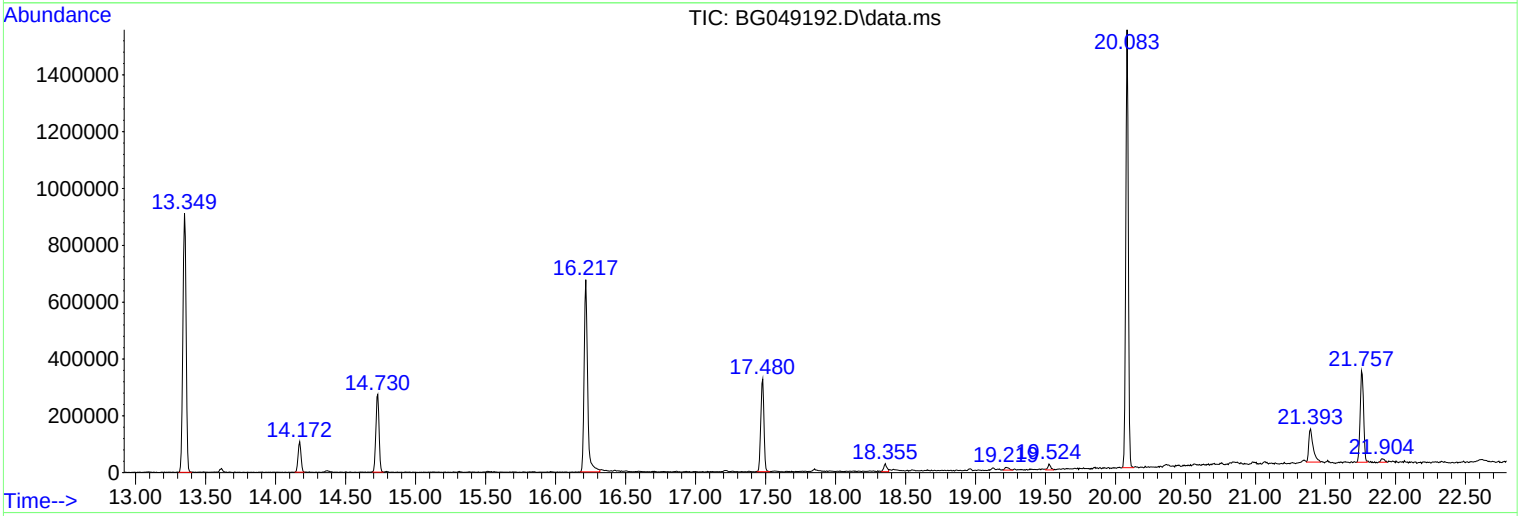
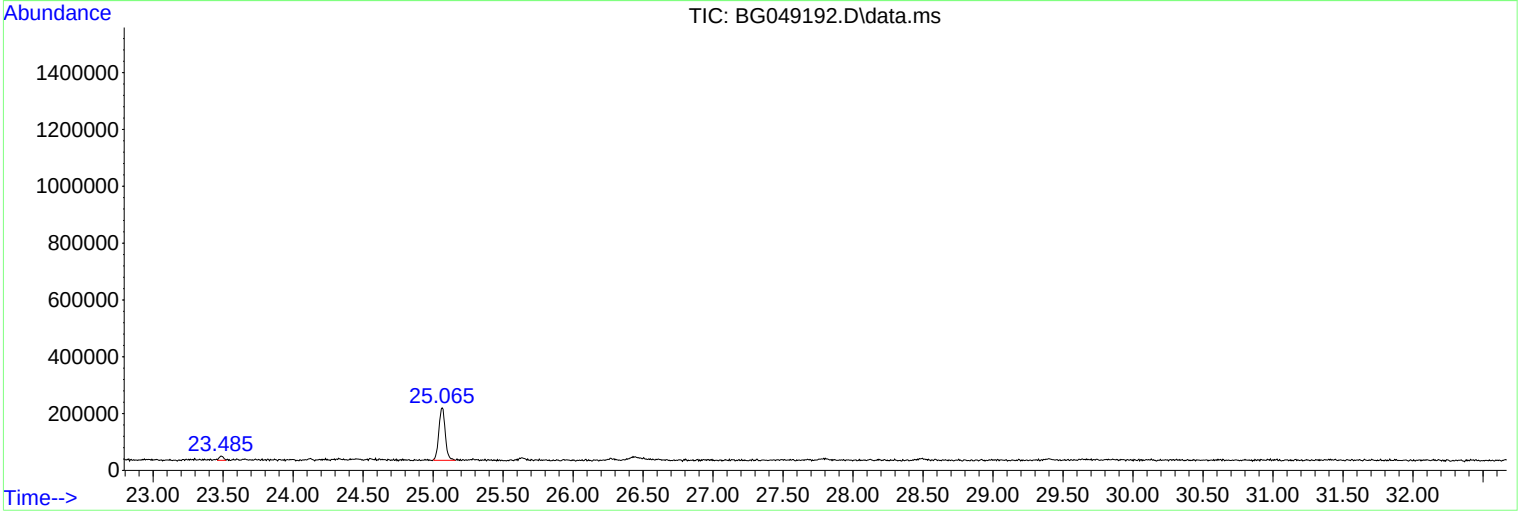
Instrument :
BNA_G
ClientSampleId :
TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.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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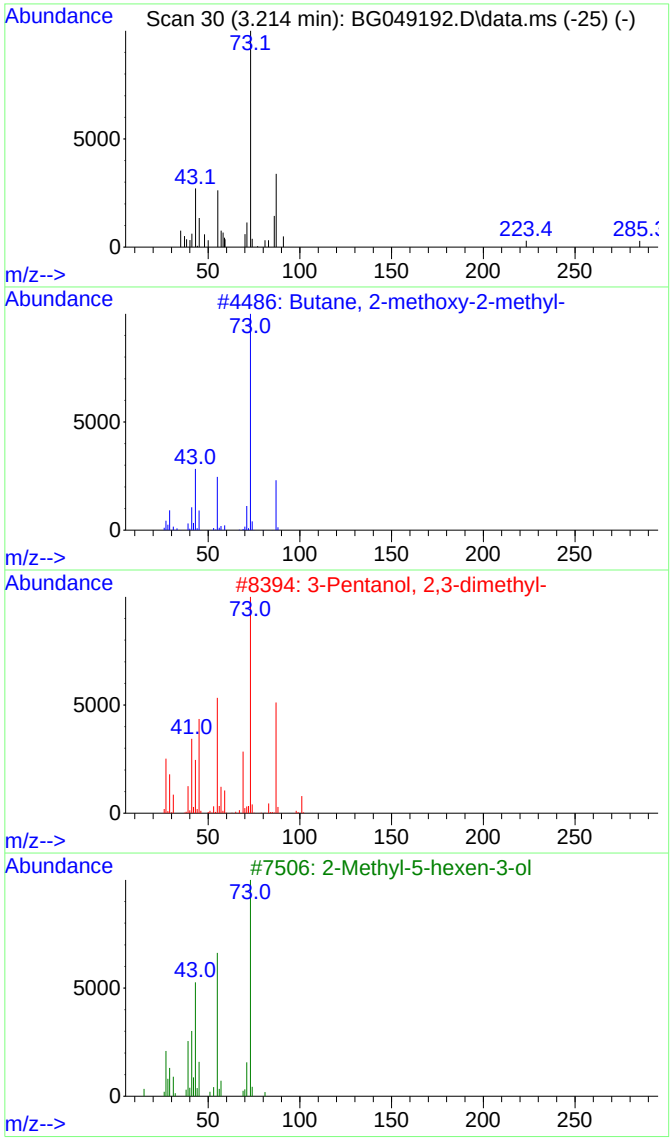
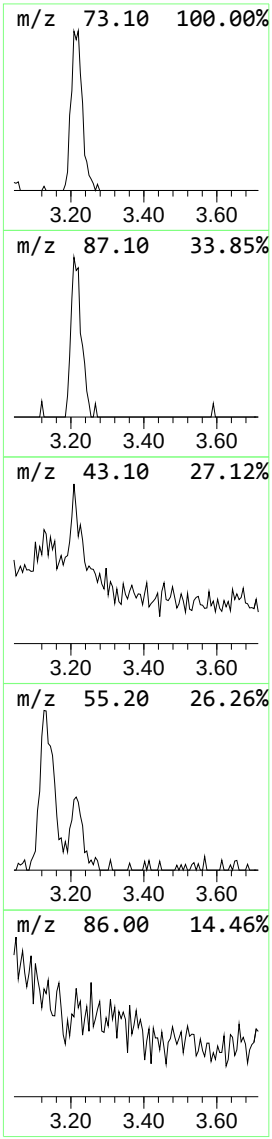
****

Peak Number 2 unknown3.214 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.214	3.30 ng	39324	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	40
2	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	9
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
4	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	9
5	3-O-Methyl-d-glucose	194	C7H14O6	1000127-25-9	9





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Sample : M2926-04
Misc :
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Instrument : BNA_G
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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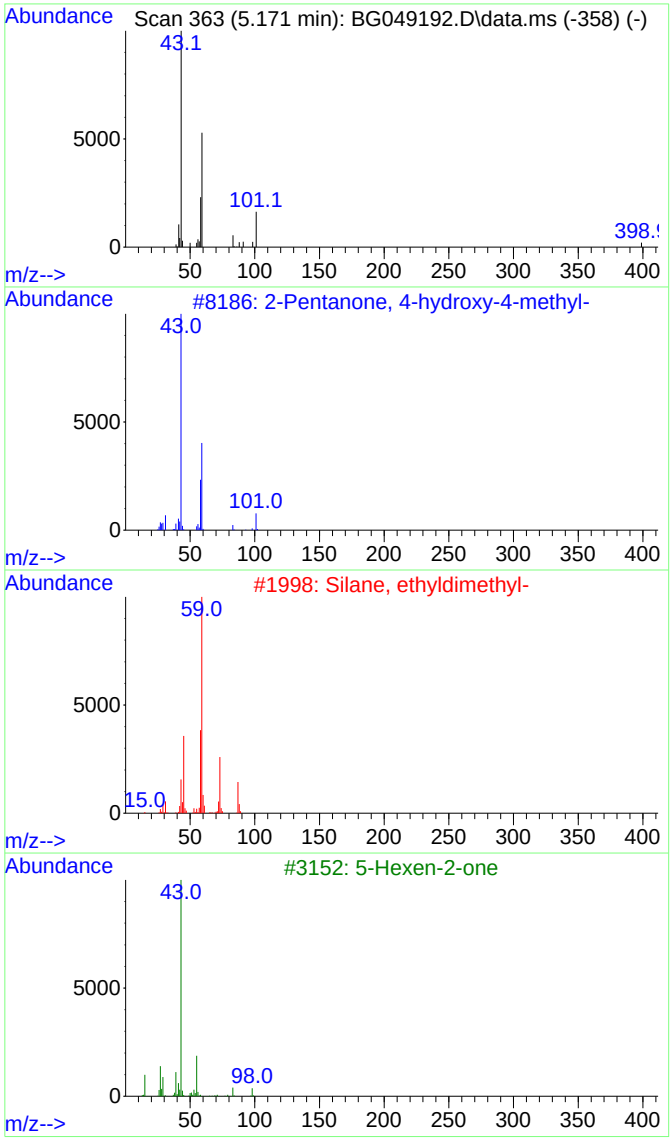
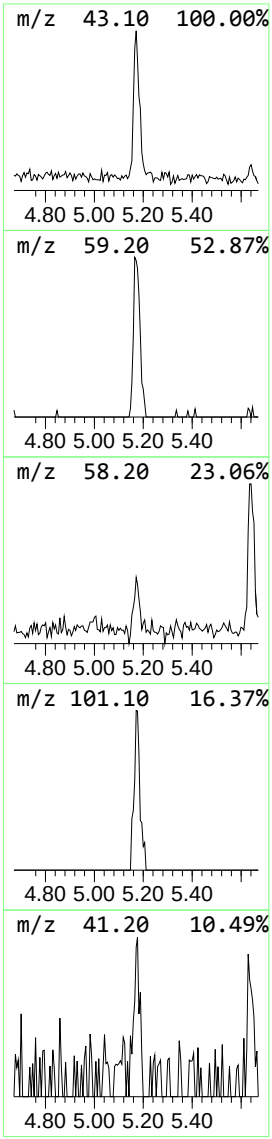
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.171	2.61 ng	31131	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	37
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	9
5	4-[(7-Hydroxy-4-oxy)heptoxy]acet...	252	C14H20O4	1000327-14-8	9





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Sample : M2926-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
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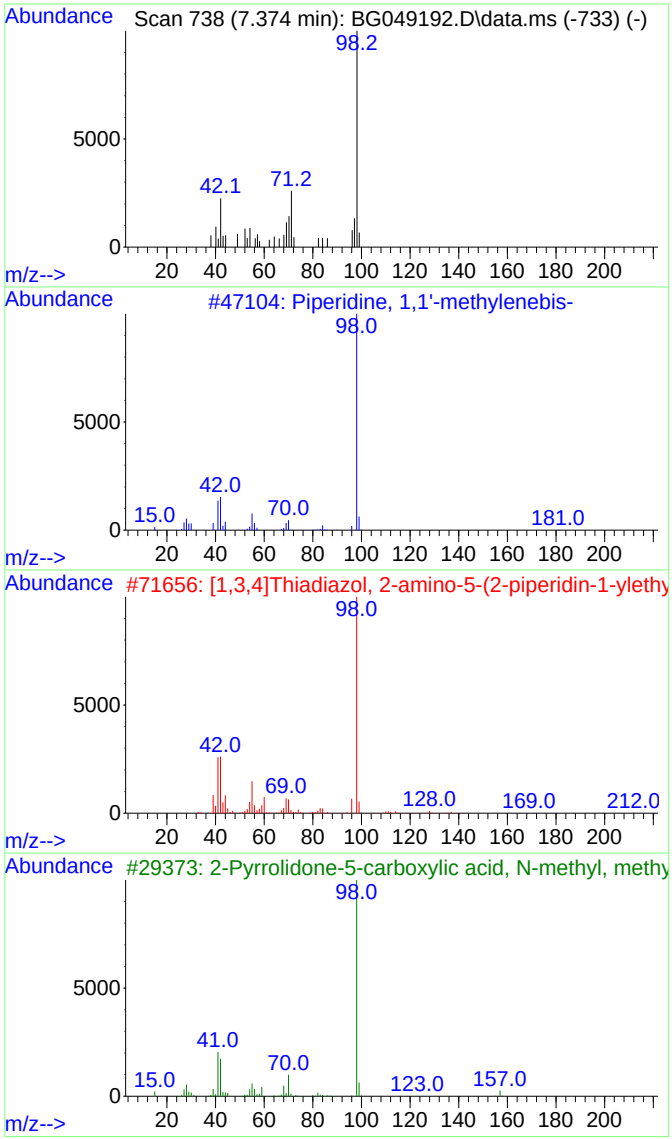
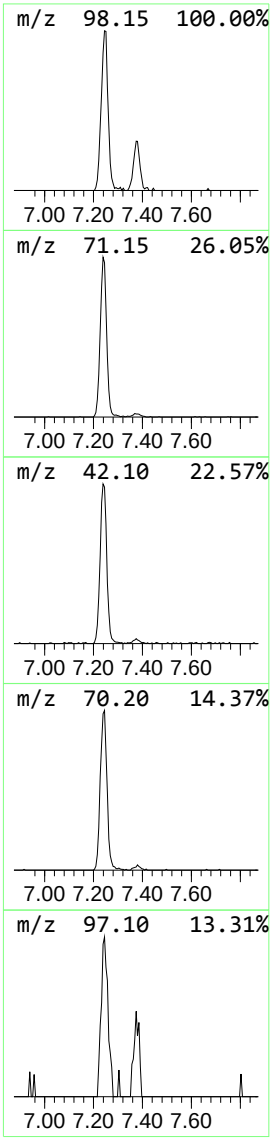
****
Peak Number 4 Piperidine, 1,1'-methylenebis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.374	2.11 ng	25174	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidine, 1,1'-methylenebis-	182	C11H22N2	000880-09-1	53
2	[1,3,4]Thiadiazol, 2-amino-5-(2-...	212	C9H16N4S	1000303-12-6	53
3	2-Pyrrolidone-5-carboxylic acid,...	157	C7H11NO3	1000333-16-8	50
4	3H-Pyrazol-3-one, 1,2-dihydro-5-...	98	C4H6N2O	004344-87-0	50
5	1,2-Cyclopentanedione	98	C5H6O2	003008-40-0	50





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Instrument : BNA_G
ClientSampleId : TP-2

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TIC Library : C:\Database\NIST11.L
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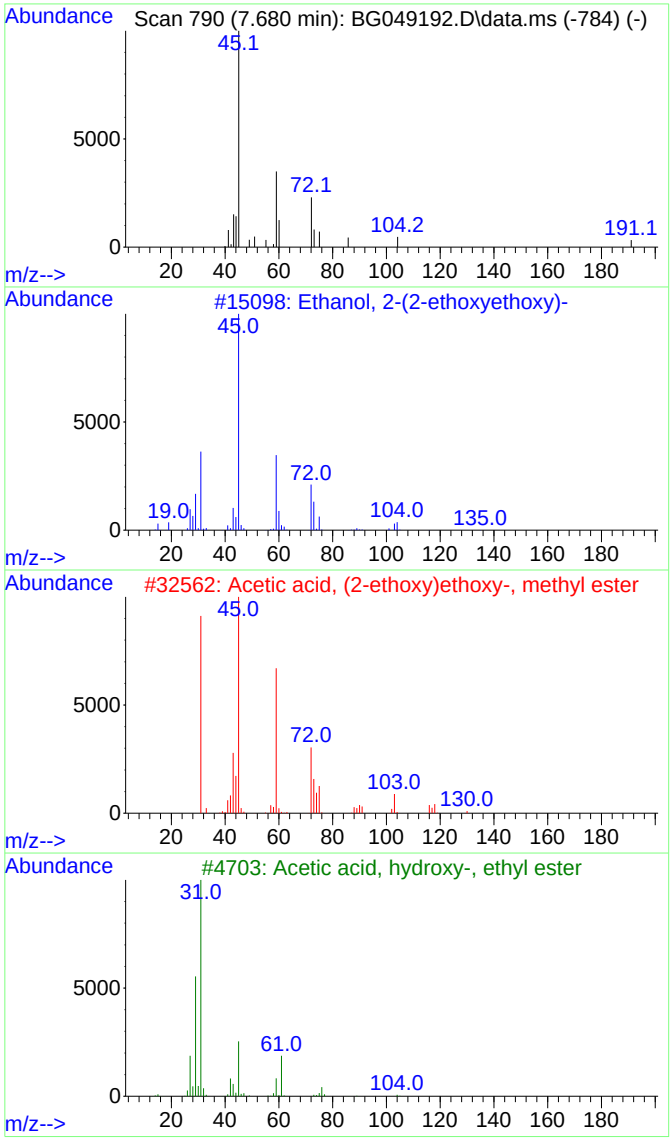
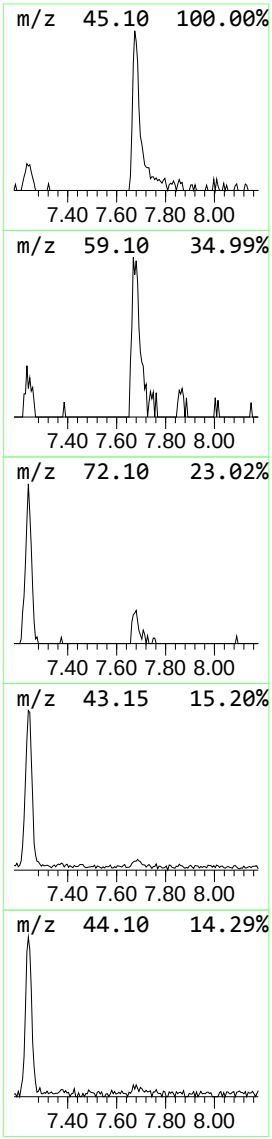
Peak Number 5 unknown7.680 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.680	2.27 ng	27018	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	40
2	Acetic acid, (2-ethoxy)ethoxy-, ...	162	C7H14O4	016326-34-4	28
3	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9
4	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	9
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9





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Instrument : BNA_G
ClientSampleId : TP-2

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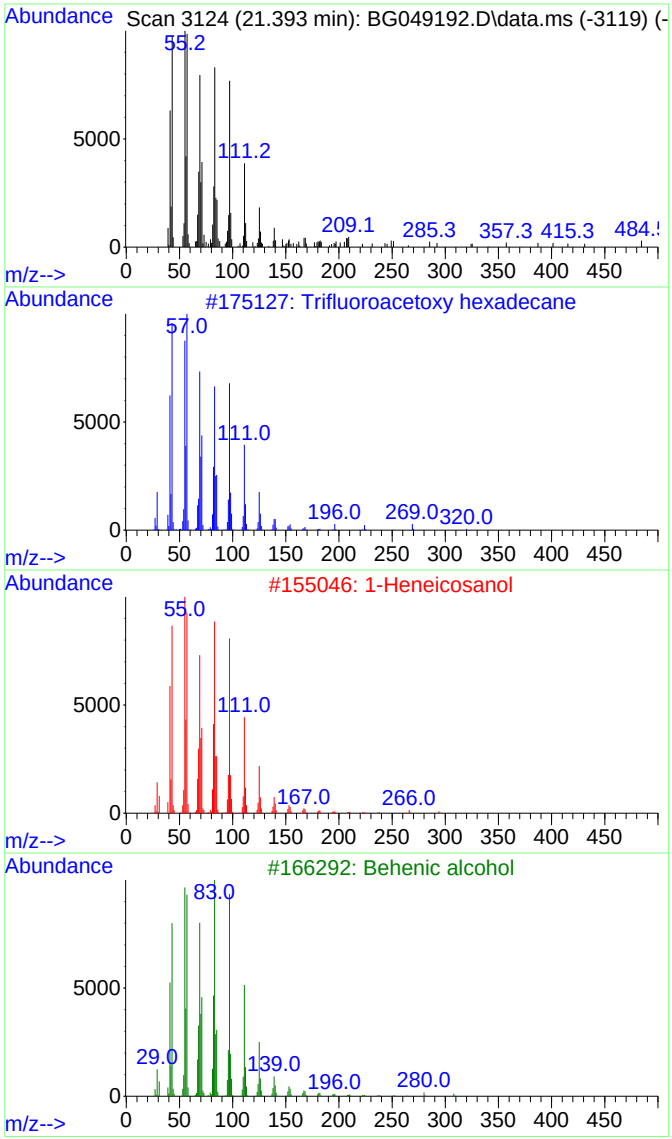
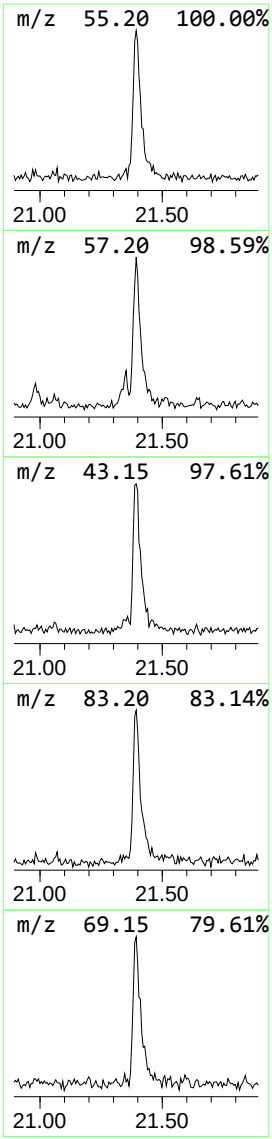
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.393	9.13 ng	245327	Chrysene-d12	21.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Docosene	308	C22H44	001599-67-3	90
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.214	3.214	3.3	ng	39324	1	8.085	238191	20.0
2-Pentanone, 4-...	5.171	2.6	ng	31131	1	8.085	238191	20.0
Piperidine, 1,1...	7.374	2.1	ng	25174	1	8.085	238191	20.0
unknown7.680	7.680	2.3	ng	27018	1	8.085	238191	20.0
Trifluoroacetox...	21.393	9.1	ng	245327	5	21.757	537304	20.0