

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120117\
 Data File : BG031333.D
 Acq On : 2 Dec 2017 00:39
 Operator : SJ/JU
 Sample : I6653-06
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-4

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.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	5.204	321	326	337	rVB3	42598	71590	1.10%	0.284%
2	5.686	402	408	424	rBV	515688	916577	14.08%	3.639%
3	7.296	672	682	692	rBV	310840	606533	9.31%	2.408%
4	7.660	737	744	765	rVB	924114	1708223	26.23%	6.782%
5	8.130	816	824	831	rBV	203183	370524	5.69%	1.471%
6	8.453	867	879	891	rBV	900247	1646712	25.29%	6.538%
7	9.300	1014	1023	1042	rBV	642175	1269334	19.49%	5.039%
8	10.945	1295	1303	1318	rBV	271237	558257	8.57%	2.216%
9	11.785	1436	1446	1454	rBV6	59907	193036	2.96%	0.766%
10	11.902	1462	1466	1479	rVB3	26091	65445	1.01%	0.260%
11	13.371	1709	1716	1736	rBV	2167840	3543707	54.42%	14.069%
12	14.752	1944	1951	1961	rVB2	487293	836296	12.84%	3.320%
13	16.238	2197	2204	2223	rBV	1729756	2822978	43.35%	11.208%
14	17.490	2410	2417	2432	rBV2	770223	1167729	17.93%	4.636%
15	20.081	2852	2858	2869	rBV	4772984	6511905	100.00%	25.853%
16	21.761	3137	3144	3161	rVB	864275	1491370	22.90%	5.921%
17	25.058	3694	3705	3717	rBV2	487356	1407534	21.61%	5.588%

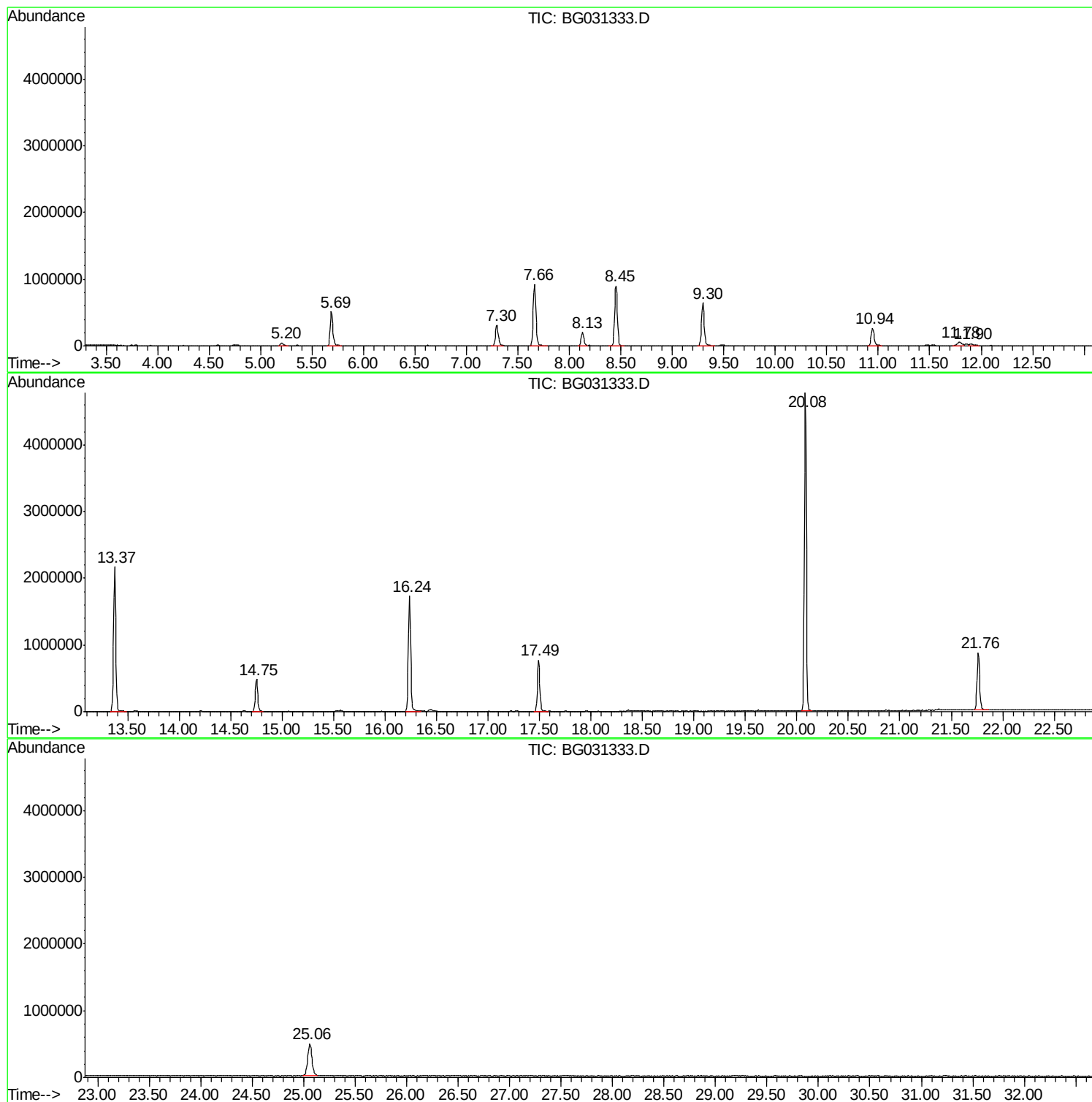
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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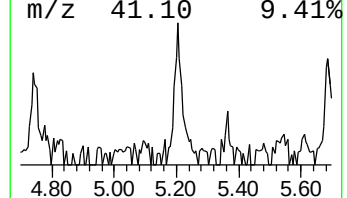
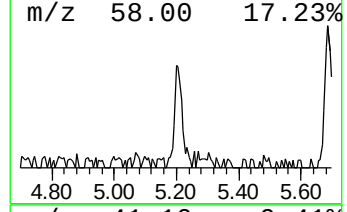
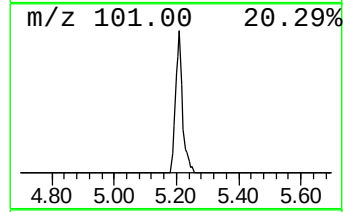
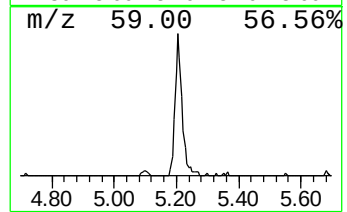
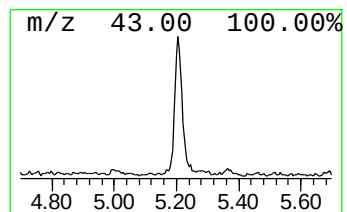
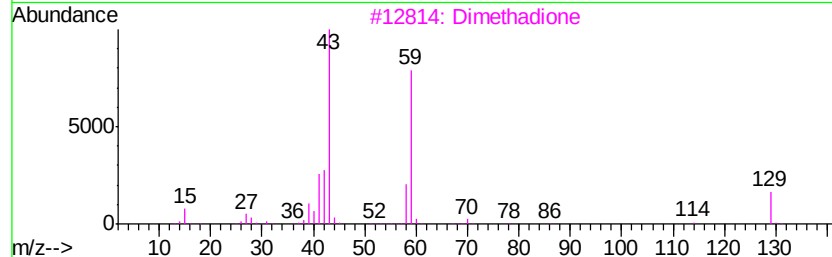
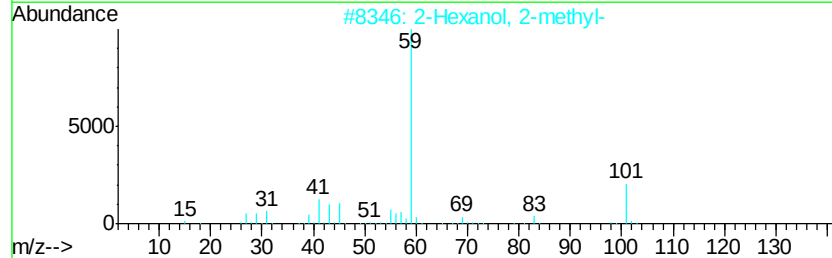
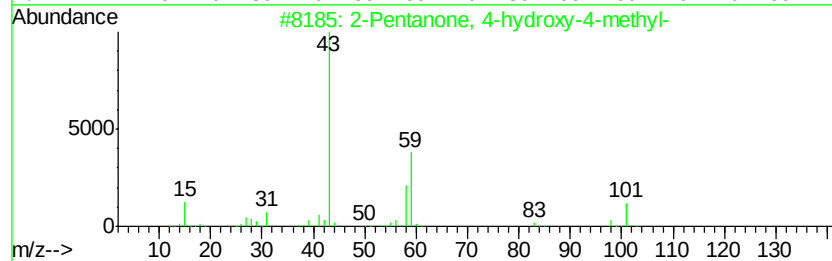
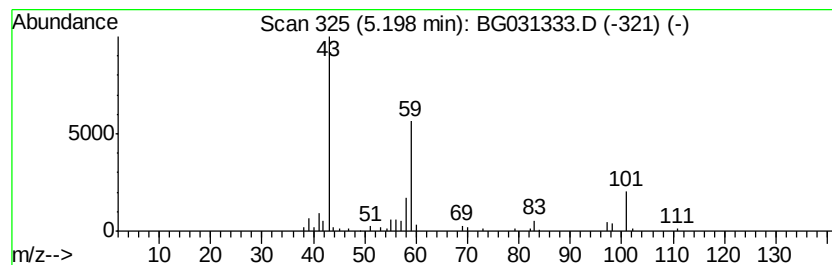
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.86 ng	71590	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			Dimethadione	129	C5H7N03	000695-53-4	28
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	27
5			2,3-Butanedione, monooxime	101	C4H7N02	000057-71-6	25



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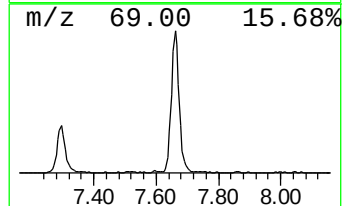
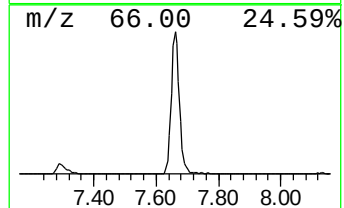
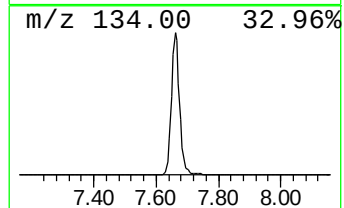
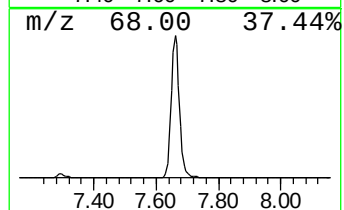
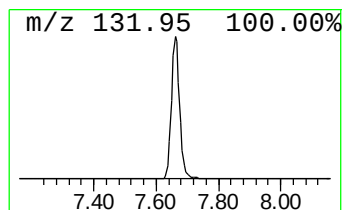
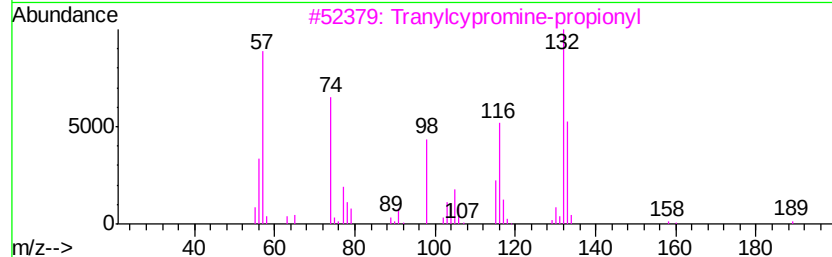
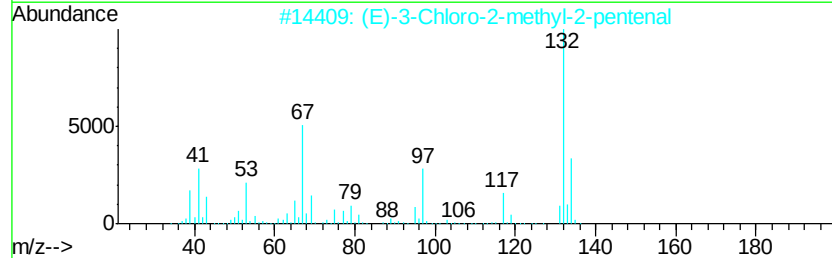
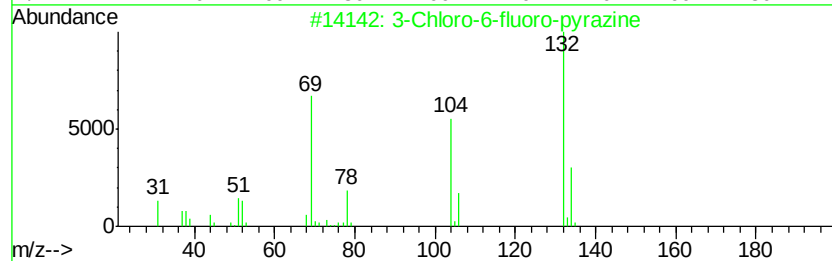
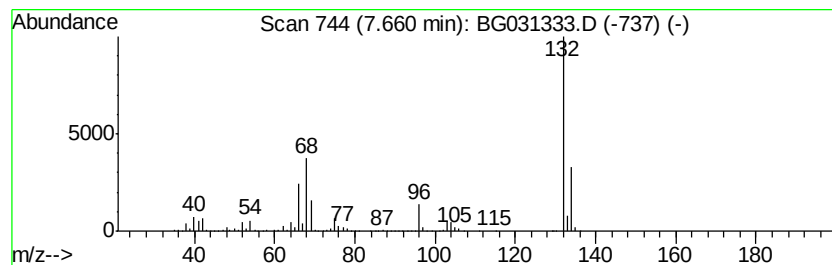
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Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	92.21 ng	1708220	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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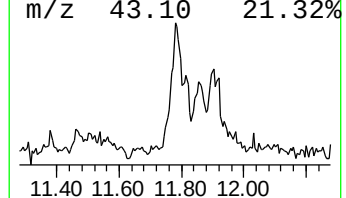
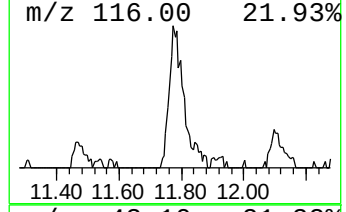
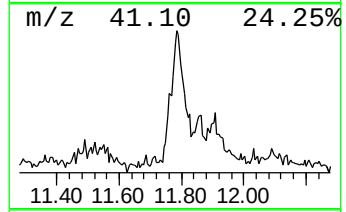
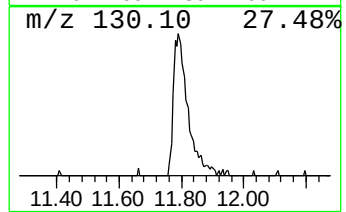
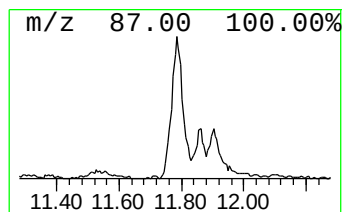
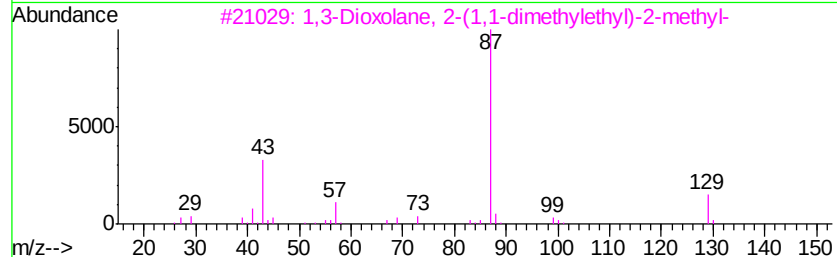
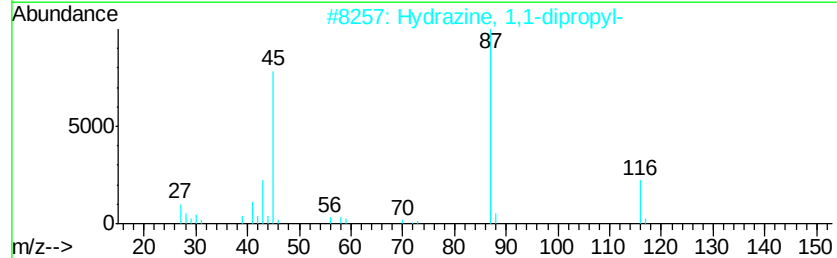
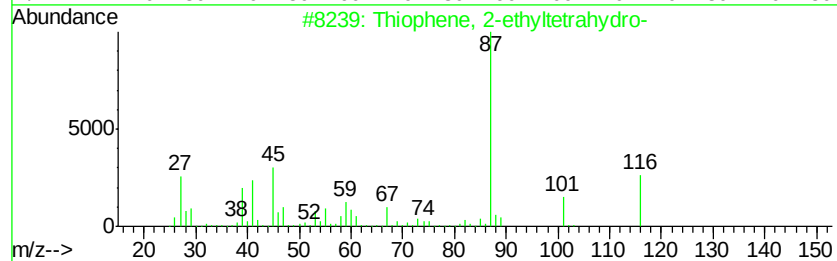
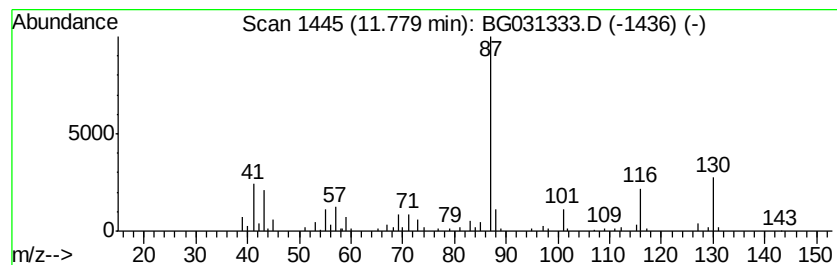
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Peak Number 4 Thiophene, 2-ethyltetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	6.92 ng	193036	Naphthalene-d8	10.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	64
2		Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	52
3		1,3-Dioxolane, 2-(1,1-dimethylethyl)-2-methyl-	144	C8H16O2	006135-54-2	50
4		Tetraethylene glycol, diacetate	278	C12H22O7	022790-12-1	43
5		2-[2-[2-[2-[2-(2-Acetyloxyethyl)-2-methyl-1,3-dioxolane-5-yl]ethoxy]ethyl]oxy]ethyl]acetate	410	C18H34O10	1000351-90-7	43



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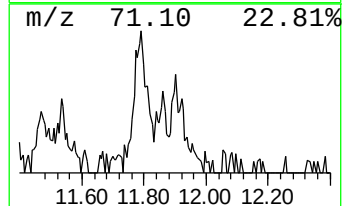
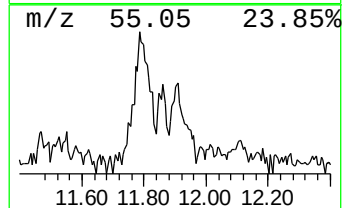
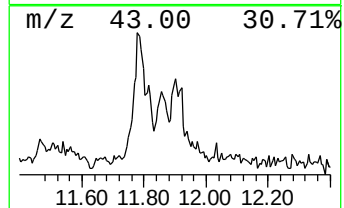
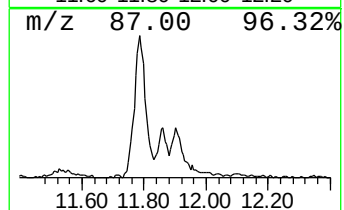
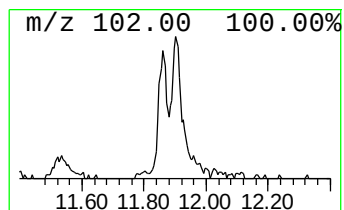
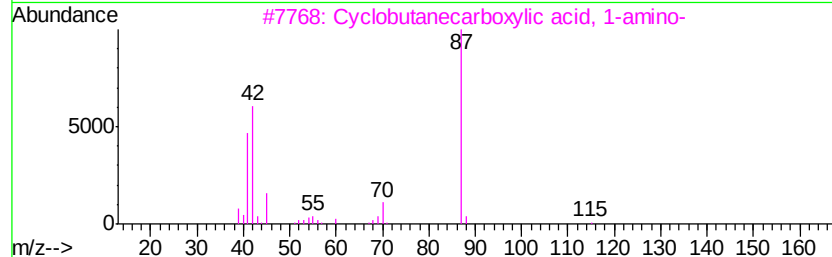
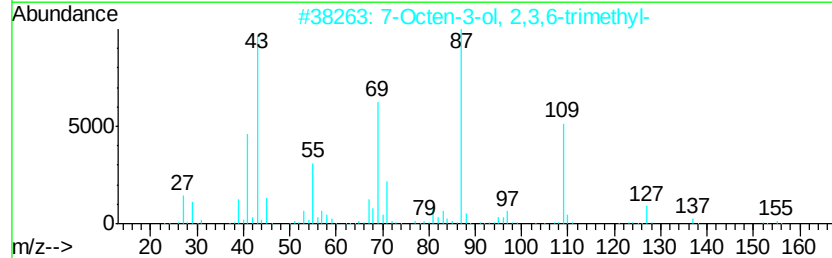
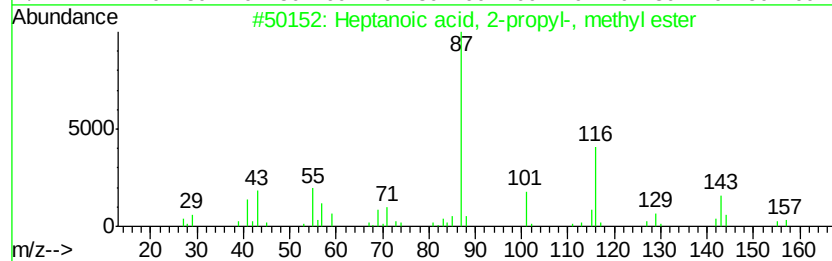
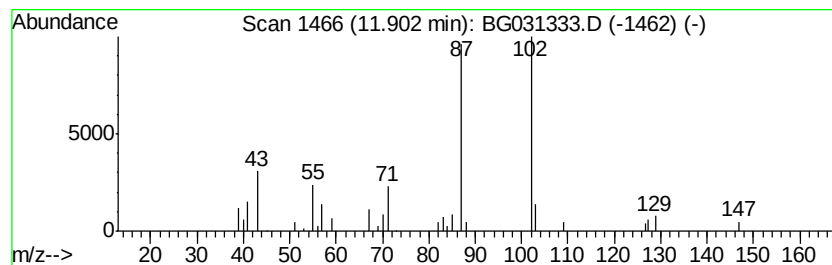
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Peak Number 5 unknown11.90 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.34 ng	65445	Naphthalene-d8	10.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptanoic acid, 2-propyl-, methyl...	186	C11H22O2	056247-53-1	25
2		7-Octen-3-ol, 2,3,6-trimethyl-	170	C11H22O	118989-21-2	17
3		Cyclobutanecarboxylic acid, 1-am...	115	C5H9NO2	022264-50-2	10
4		Cyclopropanecarboxylic acid, 6-c...	204	C10H17ClO2	1000331-01-6	10
5		4-Octanol, 4-methyl-	144	C9H20O	023418-37-3	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	3.9	ng	71590	1	8.12	370524	20.0
unknown7.66	7.66	92.2	ng	1708220	1	8.12	370524	20.0
Thiophene, 2-ethy...	11.78	6.9	ng	193036	2	10.94	558257	20.0
unknown11.90	11.90	2.3	ng	65445	2	10.94	558257	20.0