

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101221\
 Data File : BF125812.D
 Acq On : 12 Oct 2021 20:39
 Operator : JU/CG
 Sample : M4158-20
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T8-COMP-(1-4)

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_F\METHODS\8270-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125812.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.457	569	573	576	rBV	3264805	2938947	92.74%	13.585%
2	6.463	740	744	748	rBV	2707085	2734980	86.30%	12.642%
3	6.845	805	809	812	rBV	1227761	1041101	32.85%	4.812%
4	7.398	899	903	906	rBV	2019999	1742454	54.98%	8.054%
5	8.022	1006	1009	1014	rBV	486227	378709	11.95%	1.751%
6	8.122	1023	1026	1030	rVB	1641894	1256281	39.64%	5.807%
7	9.198	1205	1209	1212	rBV	4065781	3169120	100.00%	14.649%
8	9.539	1263	1267	1270	rBV3	64867	88063	2.78%	0.407%
9	9.622	1276	1281	1284	rBV2	48683	89453	2.82%	0.413%
10	9.675	1288	1290	1292	rBV2	73185	85138	2.69%	0.394%
11	9.751	1298	1303	1304	rBV3	172560	198919	6.28%	0.919%
12	9.769	1304	1306	1308	rVV	195037	162128	5.12%	0.749%
13	9.816	1312	1314	1318	rBV3	78223	103522	3.27%	0.479%
14	9.875	1318	1324	1328	rBV	1614778	1572742	49.63%	7.270%
15	9.916	1329	1331	1333	rBV3	106778	103888	3.28%	0.480%
16	9.992	1342	1344	1346	rBV2	102419	90427	2.85%	0.418%
17	10.345	1401	1404	1407	rBV4	281105	382488	12.07%	1.768%
18	10.663	1455	1458	1461	rBV	1753366	1684815	53.16%	7.788%
19	12.957	1845	1848	1852	rVB	2259507	1949146	61.50%	9.010%
20	14.004	2023	2026	2029	rVB	1242812	1014914	32.03%	4.691%
21	15.451	2268	2272	2277	rBV	740829	846701	26.72%	3.914%

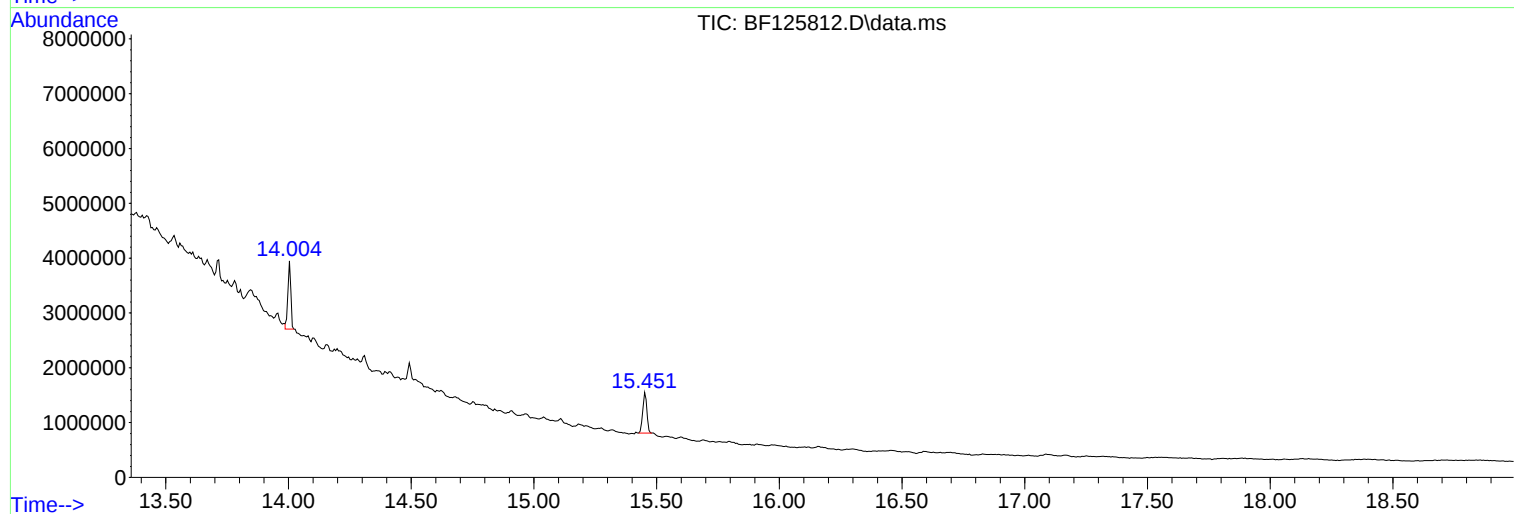
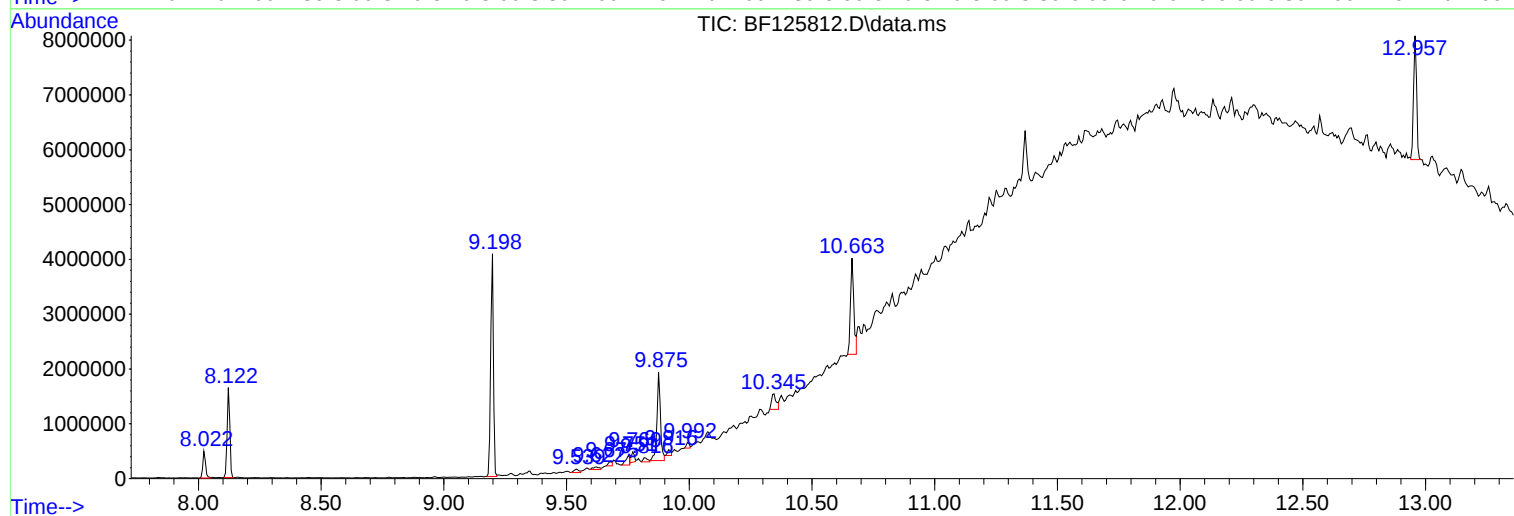
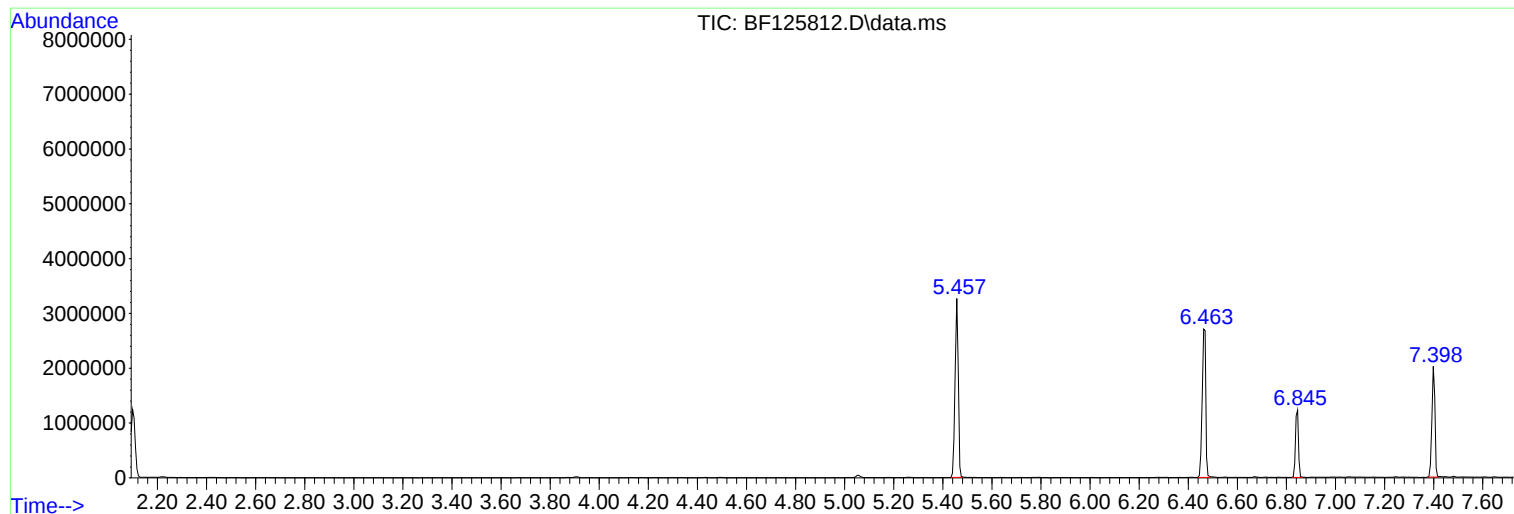
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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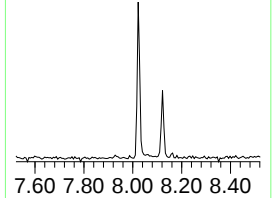
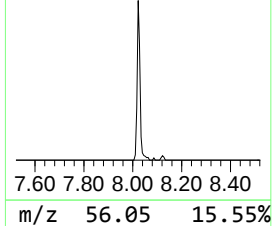
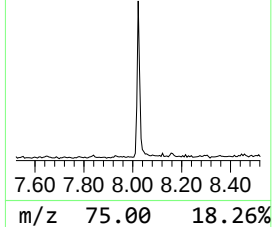
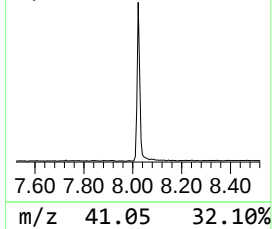
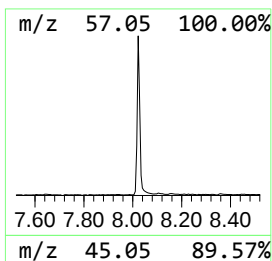
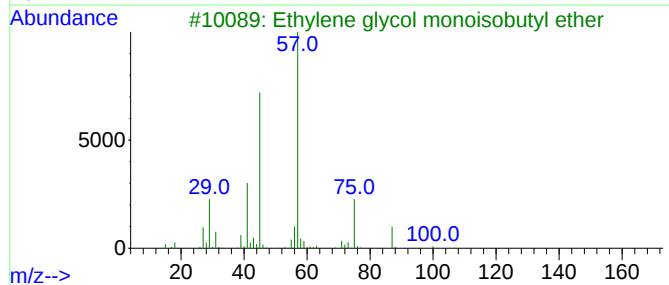
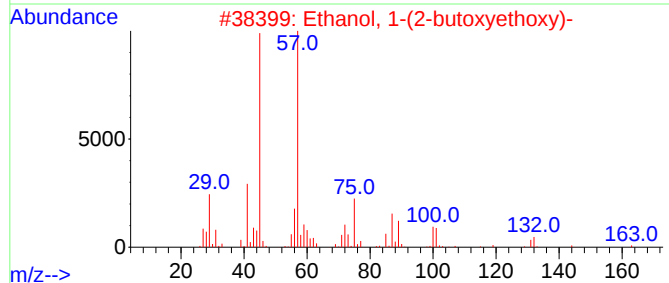
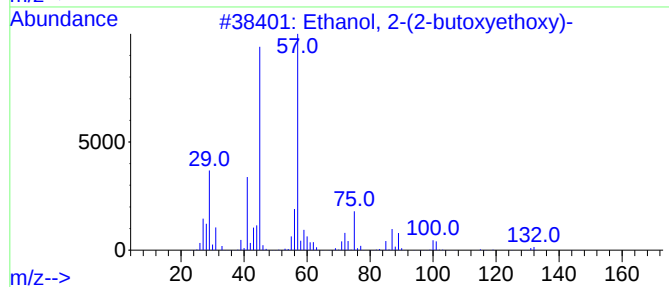
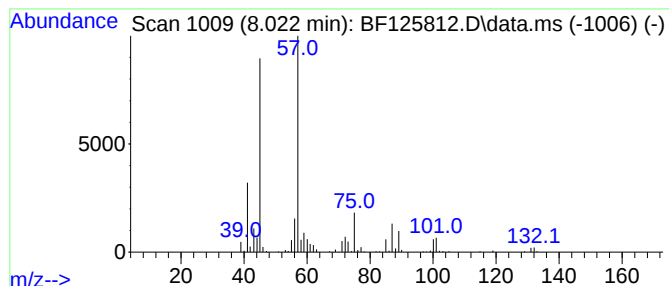
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	6.03 ng	378709	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	58
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53



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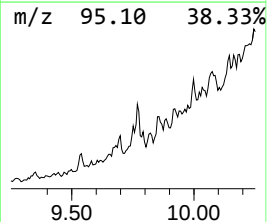
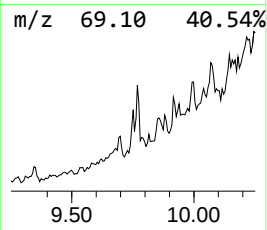
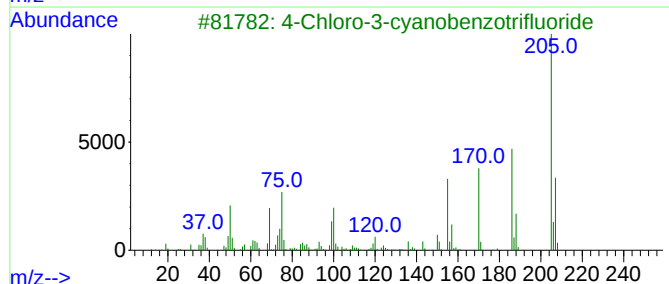
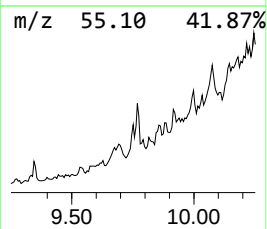
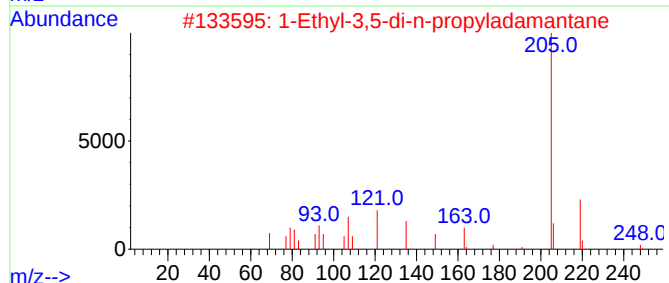
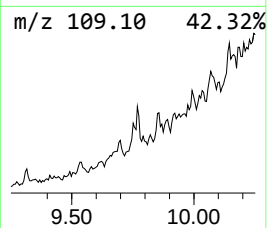
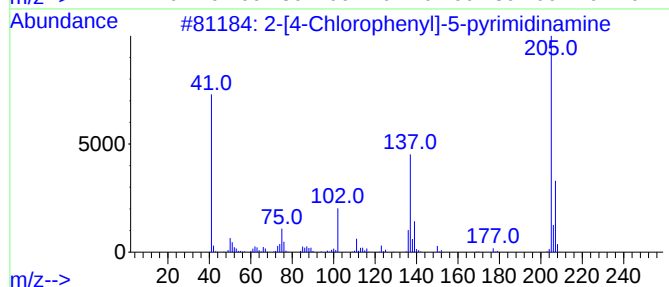
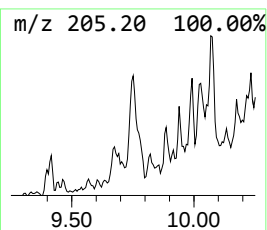
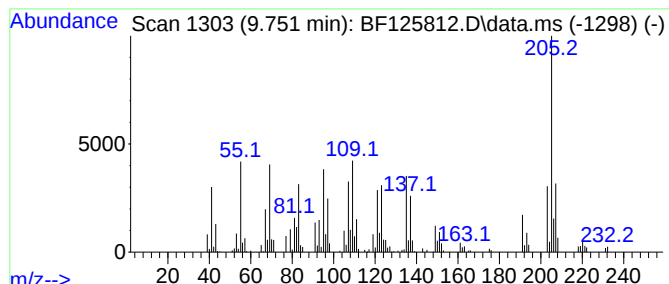
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Peak Number 2 unknown9.751 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.751	2.53 ng	198919	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		[4-Chlorophenyl]-5-pyrimidinamine	205	C10H8ClN3	1010213-57-9	35
2	1		Ethyl-3,5-di-n-propyladamantane	248	C18H32	1000215-00-4	27
3	4		Chloro-3-cyanobenzotrifluoride	205	C8H3ClF3N	000328-87-0	25
4	Phosphine,		dimenthoxy-menthyl-	480	C30H57O2P	123973-40-0	25
5	Thiazolo[5,4-d]pyrimidine,		5,7-d...	205	C5HC12N3S	013479-88-4	25



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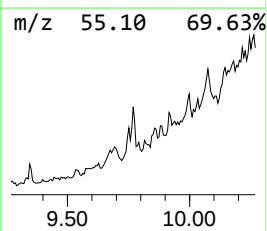
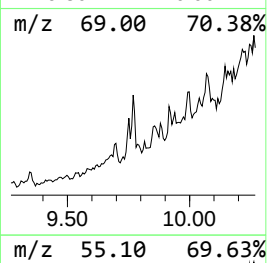
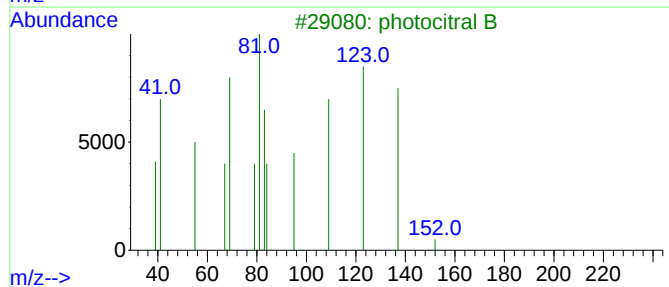
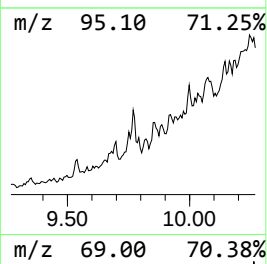
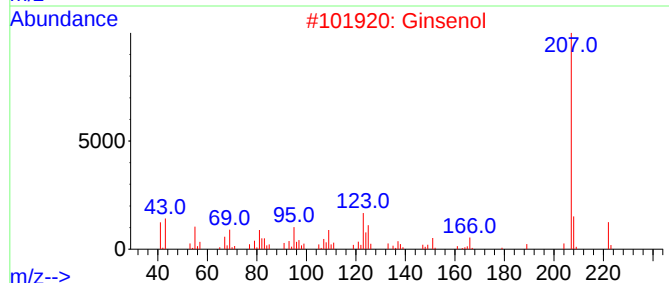
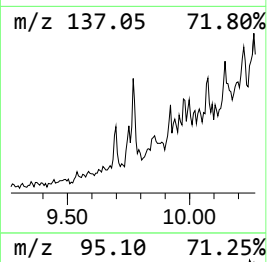
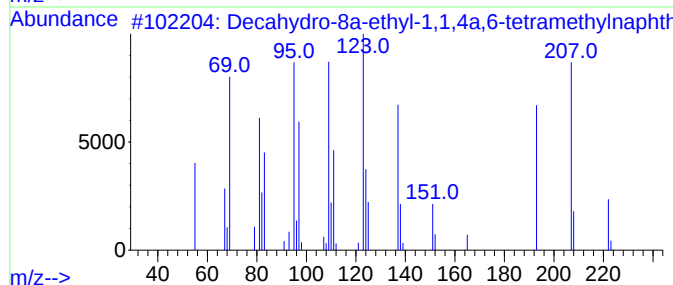
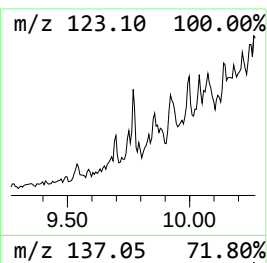
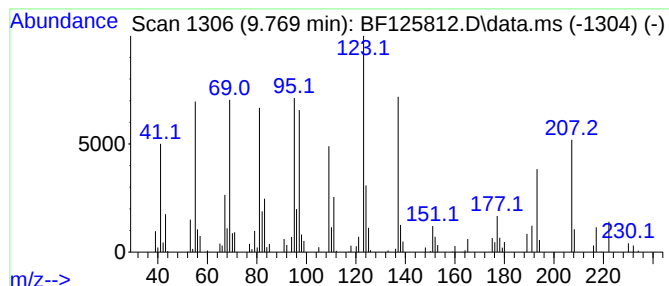
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Peak Number 3 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	2.06 ng	162128	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	98
2			Ginsenos	222	C15H26O	117591-80-7	76
3			photocitral B	152	C10H16O	006040-45-5	30
4			Butanamide, N-(2-methoxyphenyl)-...	207	C11H13NO3	000092-15-9	25
5			1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	22



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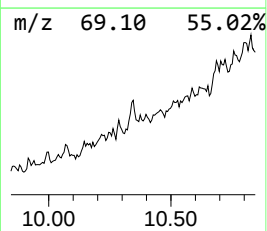
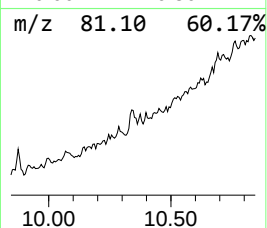
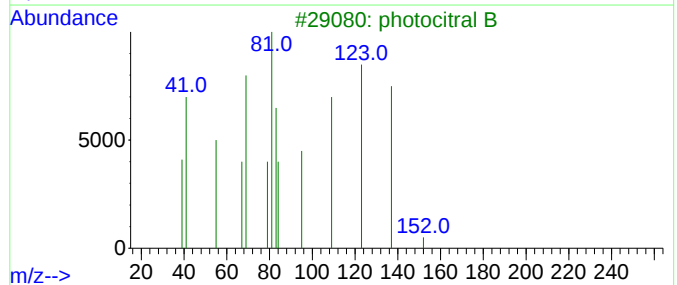
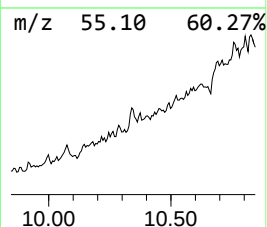
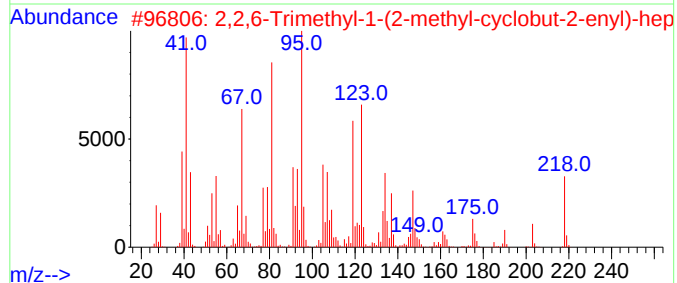
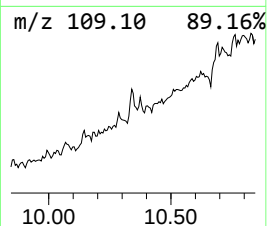
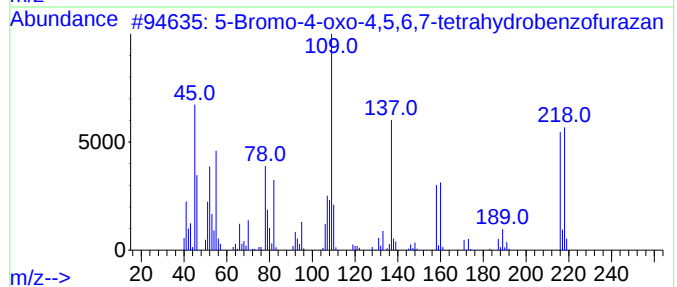
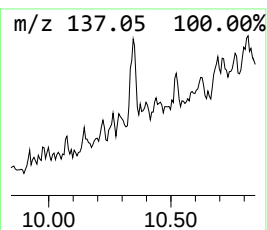
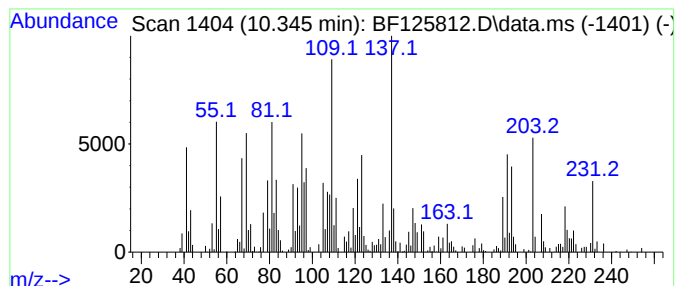
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Peak Number 4 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.345	4.86 ng	382488	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	56
2			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	42
3			photocitral B	152	C10H16O	006040-45-5	38
4			Bicyclo[2.2.1]heptan-2-one, 5-br...	230	C10H15BrO	010293-00-2	18
5			1H-Pyrrole-2,5-dione, dihydro-1-...	193	C10H11NO3	1010351-31-4	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.022	6.0	ng	378709	2	8.122	1256280	20.0
unknown9.751	9.751	2.5	ng	198919	3	9.875	1572740	20.0
Decahydro-8a-et...	9.769	2.1	ng	162128	3	9.875	1572740	20.0
5-Bromo-4-oxo-4...	10.345	4.9	ng	382488	3	9.875	1572740	20.0