

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
 Data File : BF092537.D
 Acq On : 26 Jan 2017 20:58
 Operator : SJ/MA
 Sample : I1448-05
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHA-FB012417

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_F\METHODS\8270-BF012417.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	3.595	129	132	136	rVB	35078	61091	1.16%	0.166%
2	4.510	210	212	217	rVB	80376	98464	1.87%	0.267%
3	5.150	265	268	271	rBV	364845	465641	8.87%	1.263%
4	5.561	301	304	306	rBV	2444797	2252491	42.89%	6.108%
5	6.590	391	394	396	rBV	1016679	1374144	26.16%	3.726%
6	6.739	404	407	409	rBV	3113450	3971469	75.62%	10.770%
7	6.967	425	427	430	rVB	1116097	958170	18.24%	2.598%
8	7.127	438	441	443	rBV	3738024	3481471	66.29%	9.441%
9	7.539	474	477	479	rBV	2937298	3312315	63.07%	8.982%
10	8.259	538	540	543	rVB	1237089	1234824	23.51%	3.349%
11	9.345	632	635	638	rBV	4158530	5029298	95.76%	13.638%
12	9.493	646	648	651	rBV	81021	92138	1.75%	0.250%
13	9.939	680	687	692	rBV	64615	127796	2.43%	0.347%
14	10.030	692	695	697	rVB	1611013	1495223	28.47%	4.055%
15	10.819	761	764	767	rBV	2601073	3021158	57.52%	8.193%
16	10.888	768	770	772	rVV	143201	146446	2.79%	0.397%
17	11.516	823	825	828	rVB	1693762	1465047	27.89%	3.973%
18	12.088	872	875	877	rBV2	148714	153400	2.92%	0.416%
19	13.105	961	964	967	rBV	3986291	5252047	100.00%	14.242%
20	14.065	1046	1048	1053	rBV	53204	90054	1.71%	0.244%
21	14.156	1053	1056	1058	rBV	1625297	1554568	29.60%	4.216%
22	15.642	1182	1186	1192	rVB	774686	1184087	22.55%	3.211%
23	16.122	1226	1228	1231	rVB	39580	55022	1.05%	0.149%

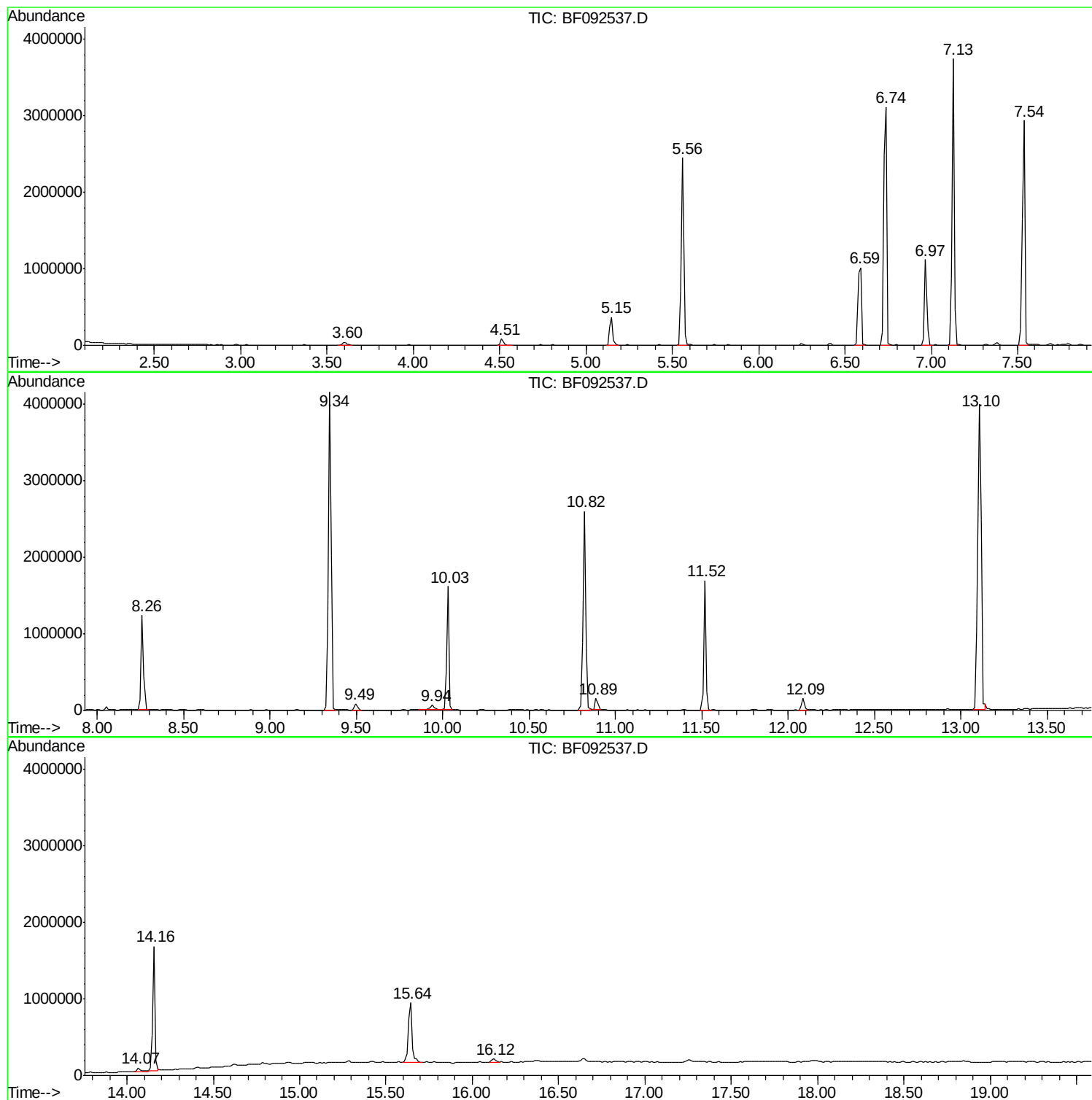
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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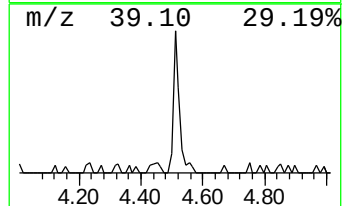
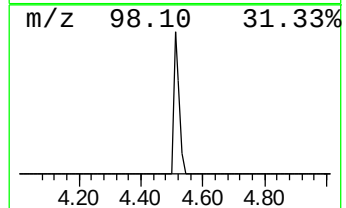
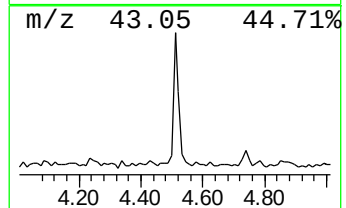
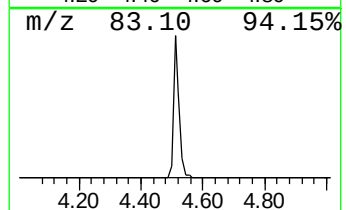
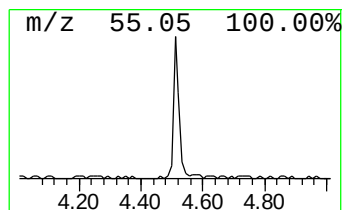
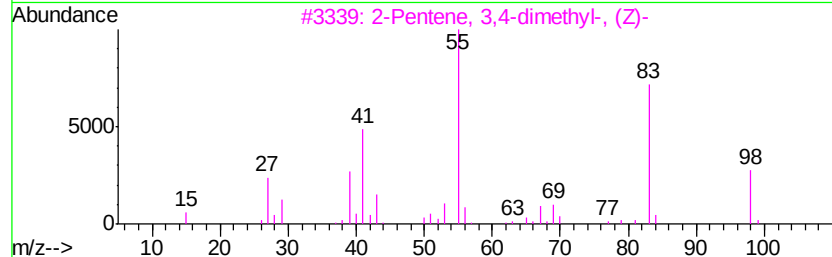
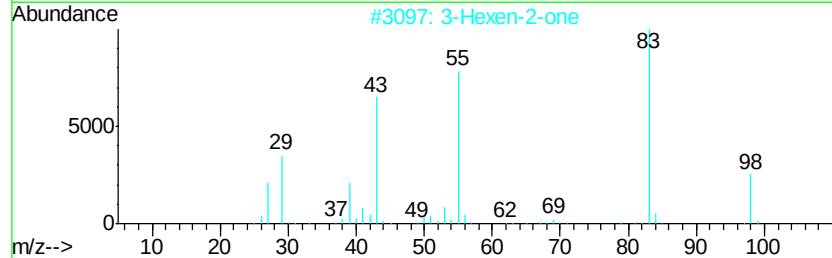
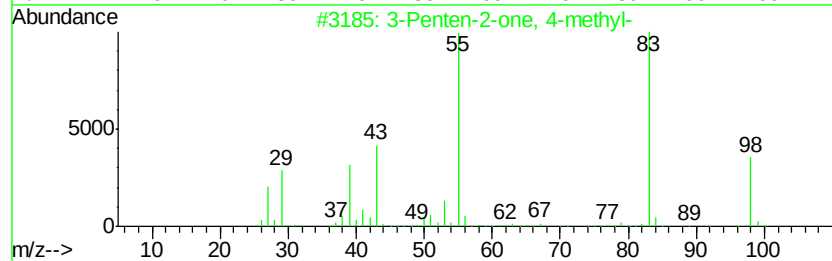
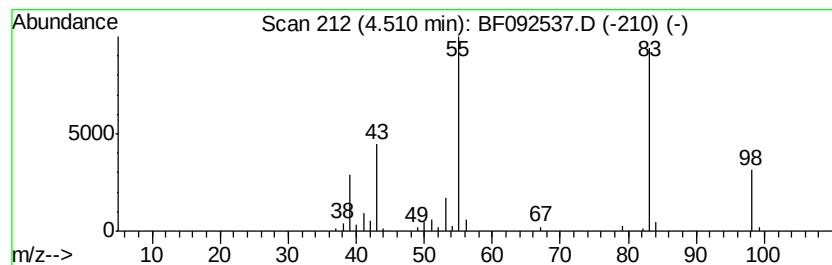
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.51	2.06 ng	98464	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	78



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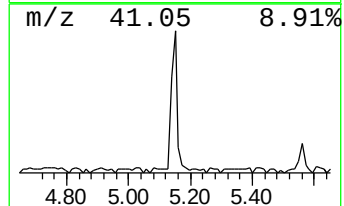
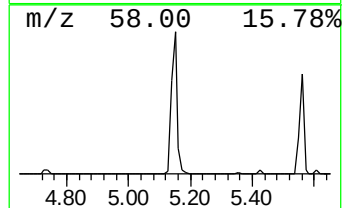
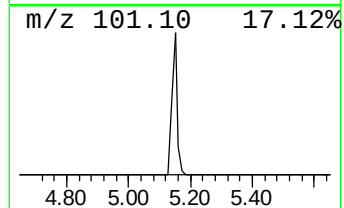
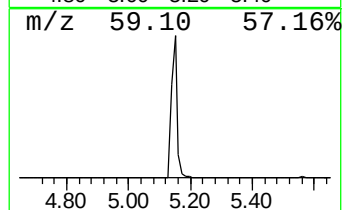
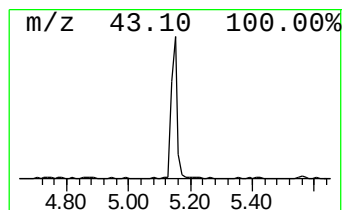
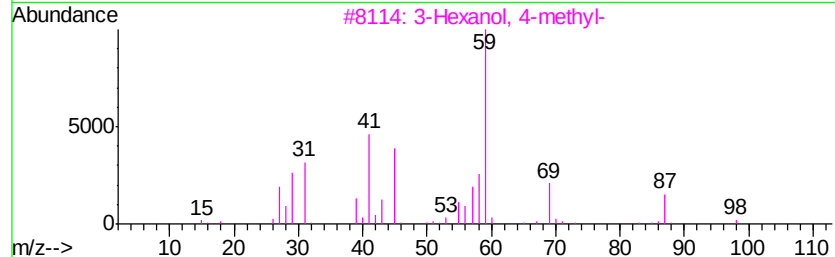
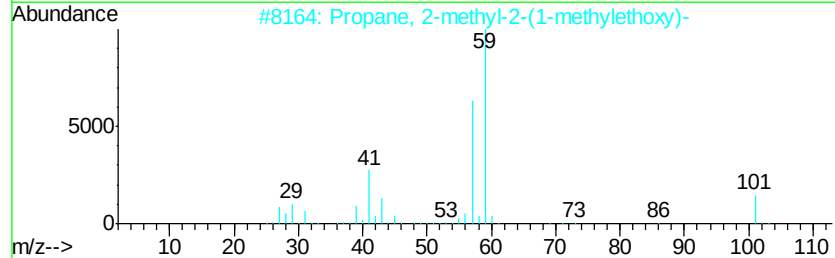
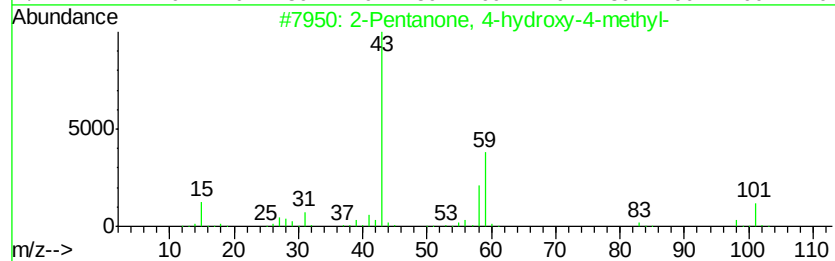
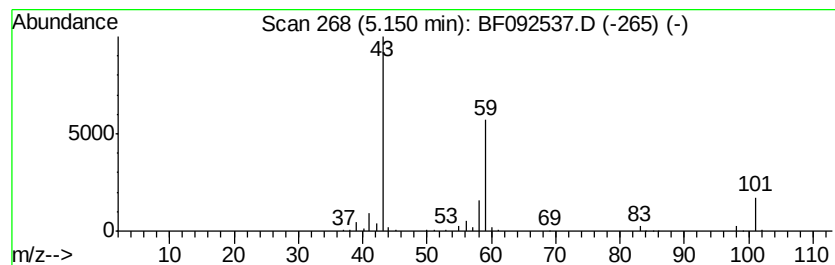
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	9.72 ng	465641	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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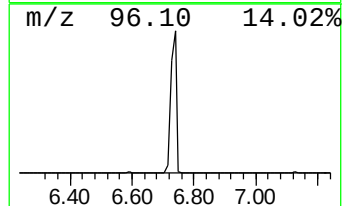
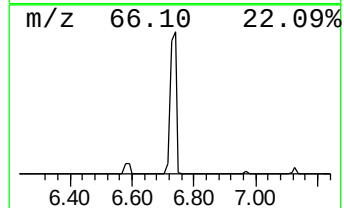
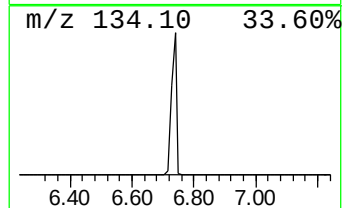
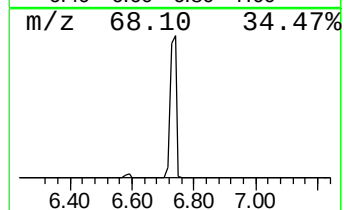
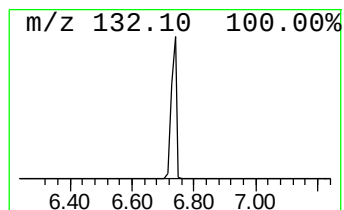
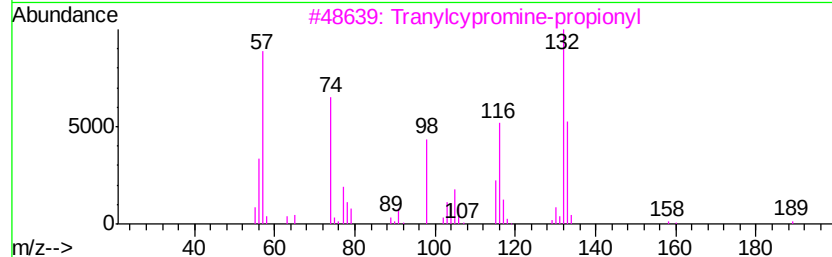
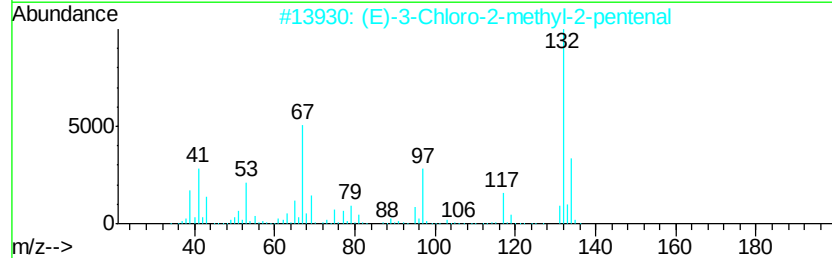
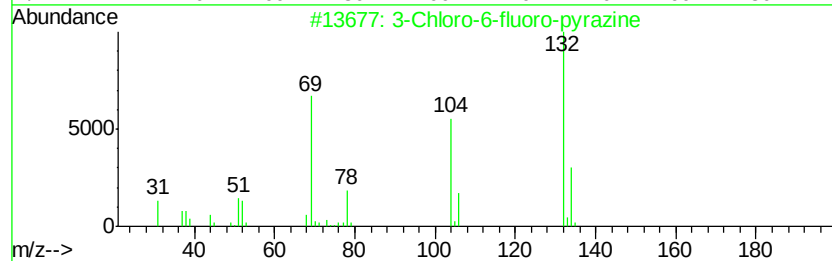
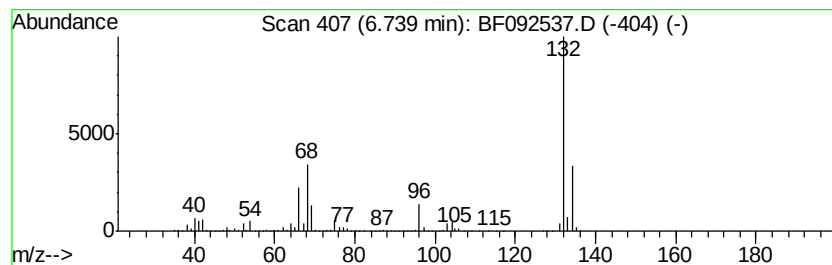
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Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	82.90 ng	3971470	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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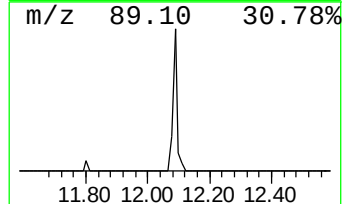
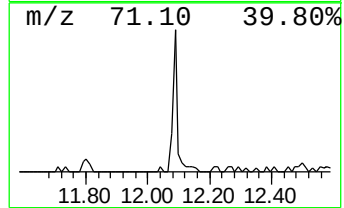
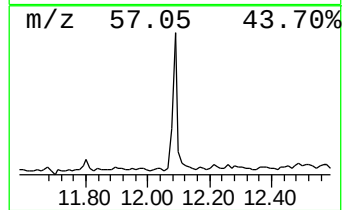
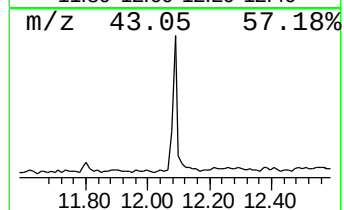
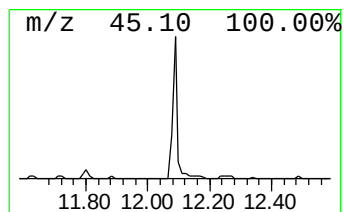
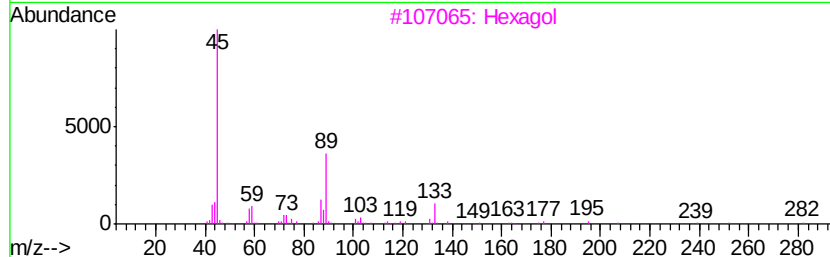
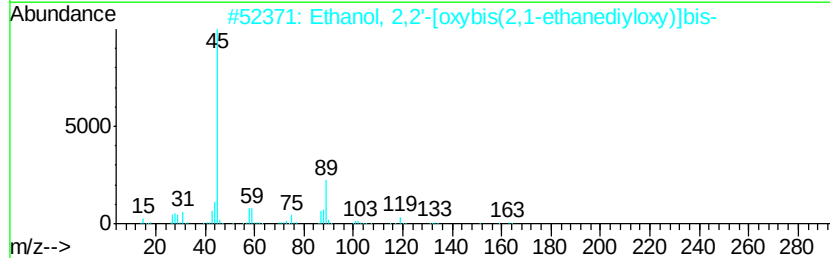
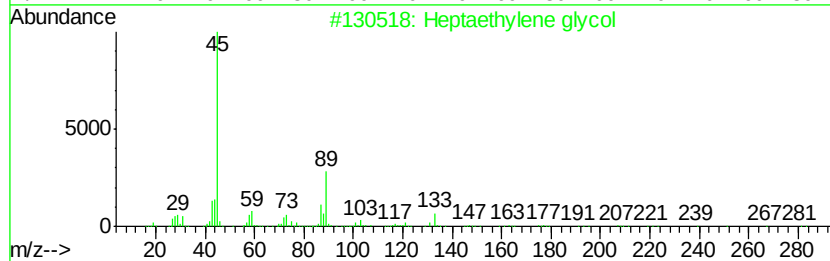
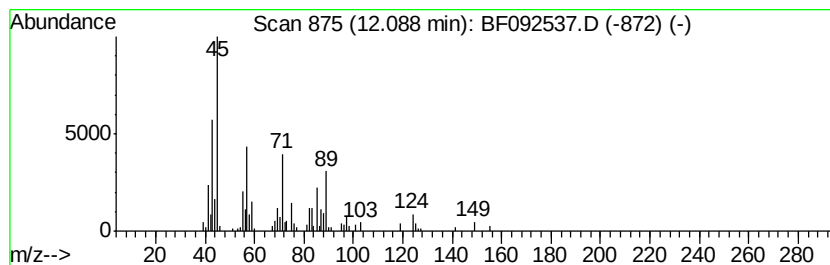
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Peak Number 5 unknown12.09 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	2.09 ng	153400	Phenanthrene-d10	11.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptaethylene glycol	326	C14H30O8	005617-32-3	49
2		Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	47
3		Hexadecol	282	C12H26O7	002615-15-8	47
4		Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	47
5		Pentaethylene glycol	238	C10H22O6	004792-15-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.51	2.1 ng		98464	1	6.97	958170	20.0
2-Pentanone, 4-hy...	5.15	9.7 ng		465641	1	6.97	958170	20.0
unknown6.74	6.74	82.9 ng		3971470	1	6.97	958170	20.0
unknown12.09	12.09	2.1 ng		153400	4	11.52	1465050	20.0