

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072715\
 Data File : BF080690.D
 Acq On : 28 Jul 2015 1:02
 Operator : TP/UM
 Sample : G3084-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUMBO-EP-1

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:\HPCHEM1\BNA_F\METHODS\8270-BF072715.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	4.453	205	207	211	rVB	12388	17812	1.77%	0.241%
2	5.093	261	263	266	rBV	562775	569267	56.66%	7.706%
3	5.504	297	299	302	rBV	905861	1004622	100.00%	13.599%
4	5.927	334	336	339	rBV	45397	41479	4.13%	0.561%
5	6.533	387	389	392	rBV	1088350	945972	94.16%	12.805%
6	6.682	400	402	405	rBV	1082399	986772	98.22%	13.358%
7	6.922	421	423	425	rBV	200012	157504	15.68%	2.132%
8	7.082	434	437	439	rVB	789821	705382	70.21%	9.549%
9	7.482	470	472	474	rBV	730241	572092	56.95%	7.744%
10	8.213	533	536	538	rBV	133322	178758	17.79%	2.420%
11	9.288	627	630	632	rVB	861026	817495	81.37%	11.066%
12	9.676	662	664	666	rVB	217079	163616	16.29%	2.215%
13	9.962	687	689	691	rBV	174028	145236	14.46%	1.966%
14	10.751	756	758	760	rBV	341835	350163	34.86%	4.740%
15	11.448	817	819	820	rBV	131505	107907	10.74%	1.461%
16	11.528	823	826	828	rVB	22499	25429	2.53%	0.344%
17	11.676	837	839	843	rBV	13851	19724	1.96%	0.267%
18	12.248	887	889	891	rBV	15715	18355	1.83%	0.248%
19	12.682	925	927	929	rVB	54969	46280	4.61%	0.626%
20	12.922	945	948	950	rVB	41573	40139	4.00%	0.543%
21	13.082	960	962	964	rVB	382651	371856	37.01%	5.034%
22	14.260	1062	1065	1067	rBV2	51810	66888	6.66%	0.905%
23	15.940	1209	1212	1214	rBV	18917	24079	2.40%	0.326%
24	16.488	1258	1260	1264	rBV3	3122	10442	1.04%	0.141%

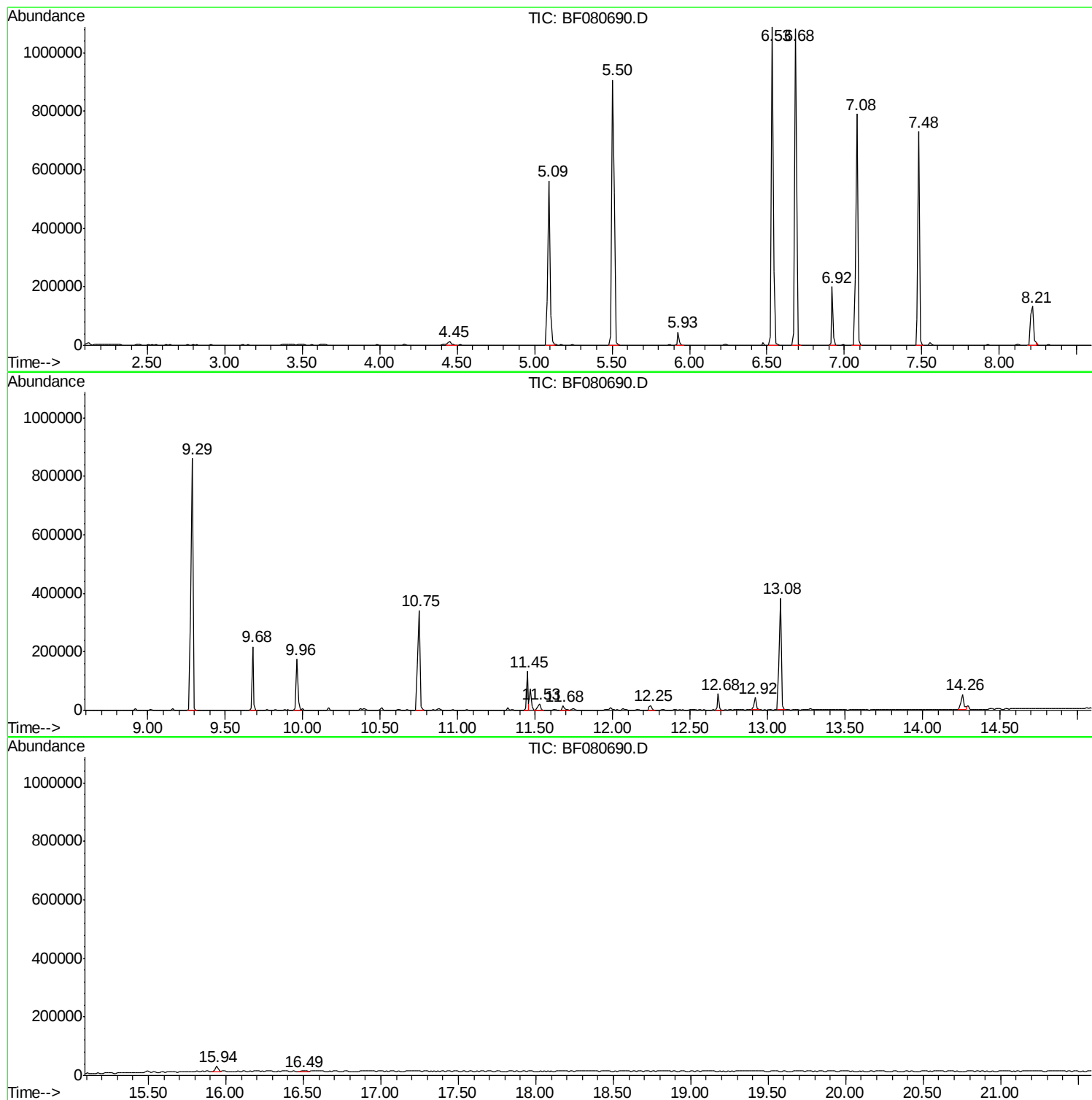
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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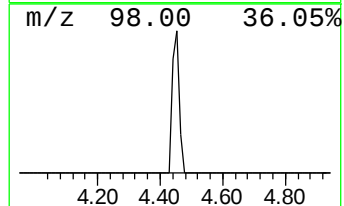
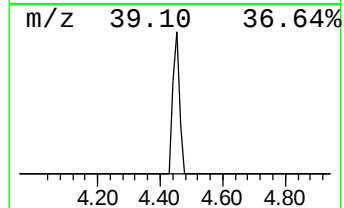
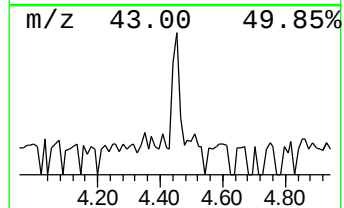
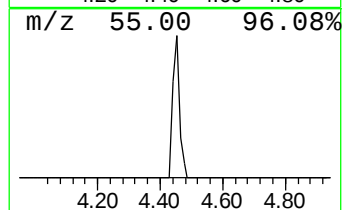
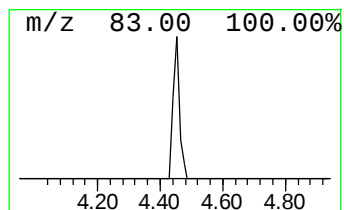
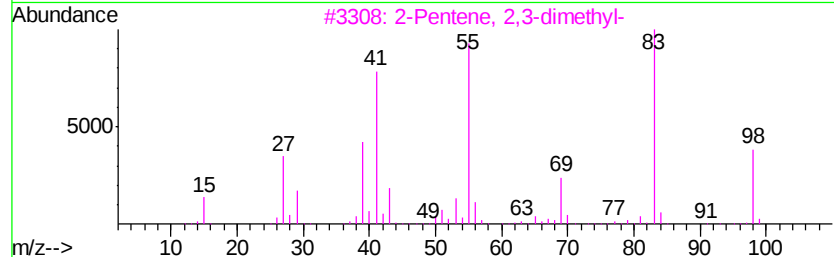
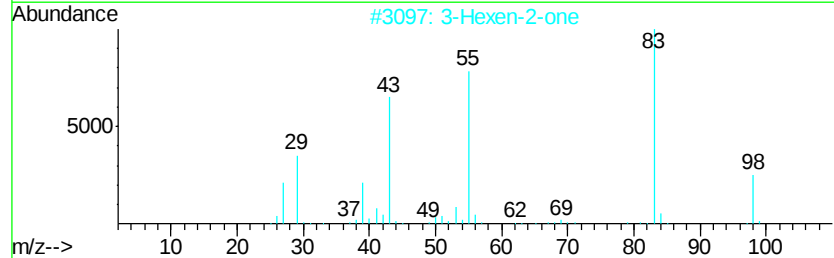
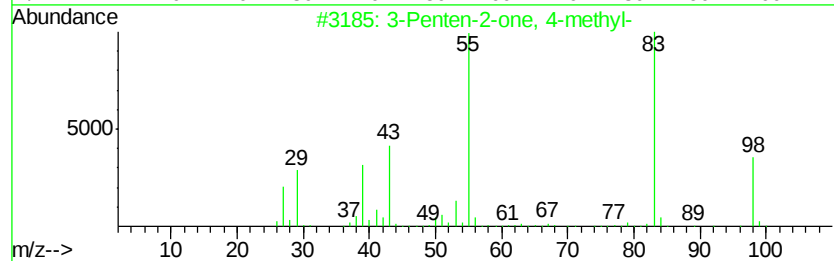
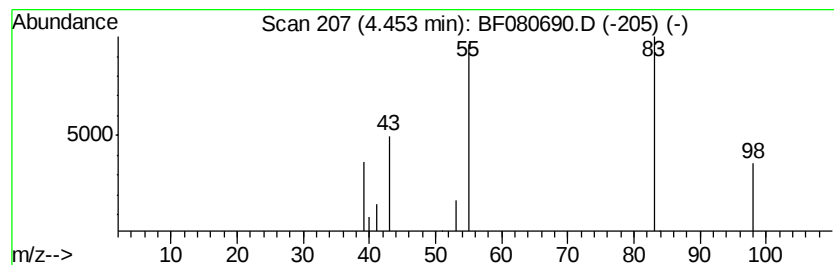
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	2.26 ng	17812	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	83
2			3-Hexen-2-one	98	C6H10O	000763-93-9	64
3			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	64
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	64
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64



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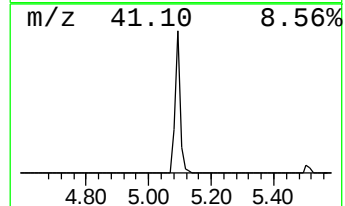
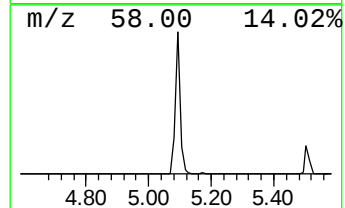
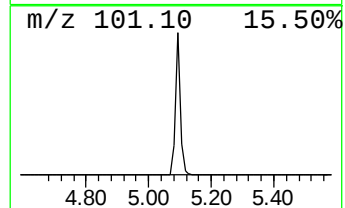
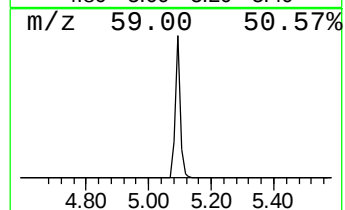
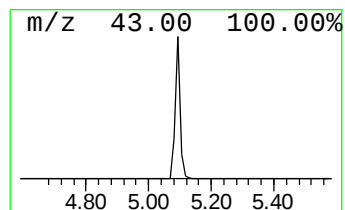
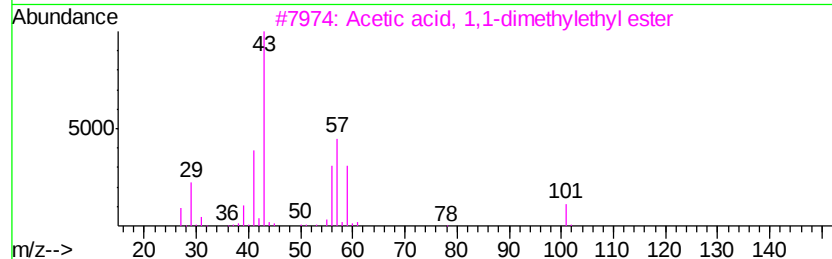
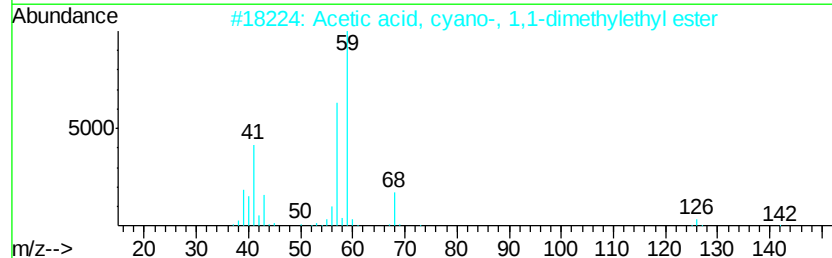
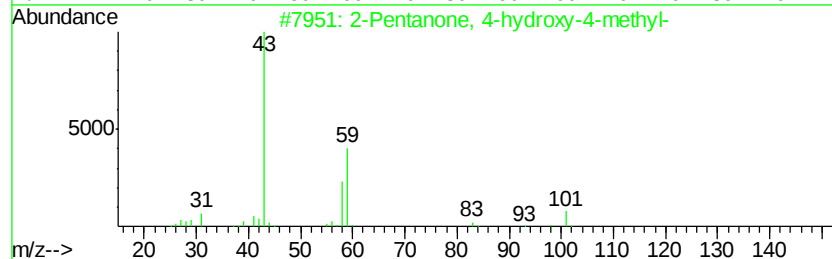
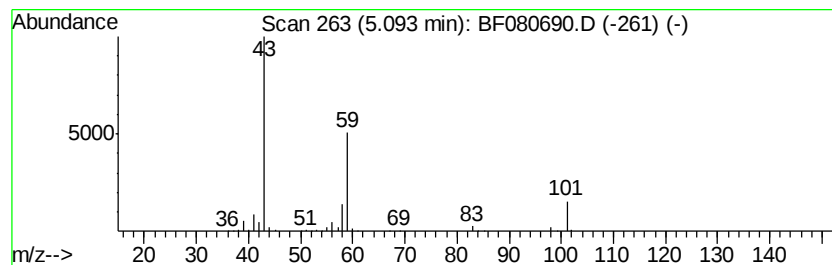
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	72.29 ng	569267	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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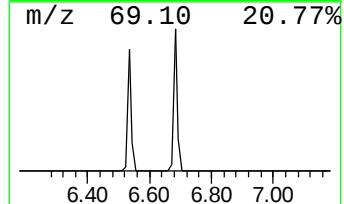
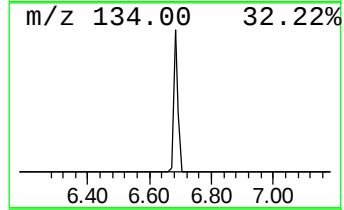
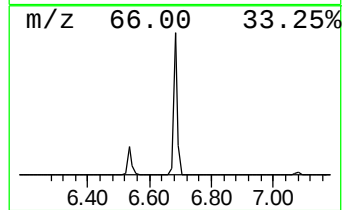
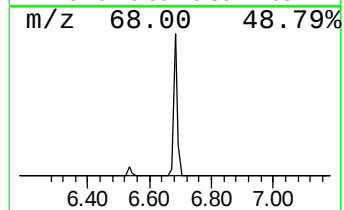
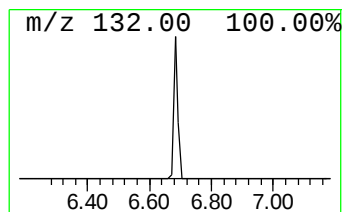
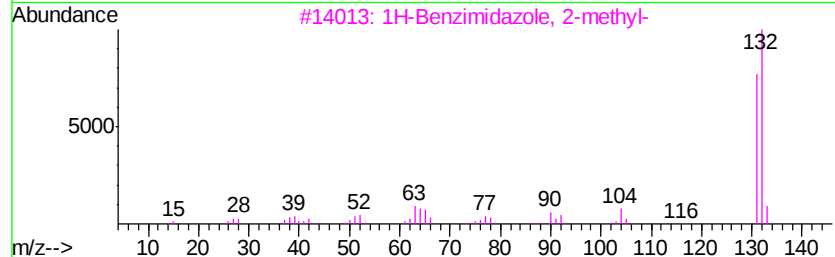
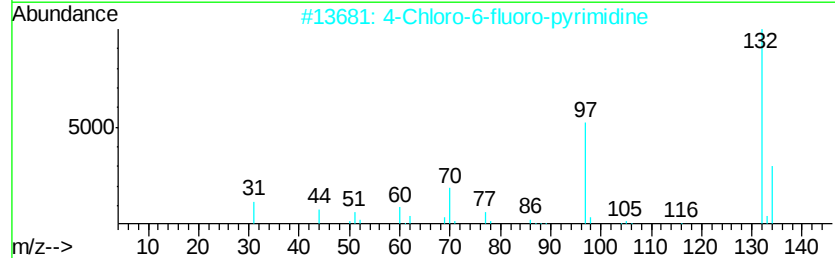
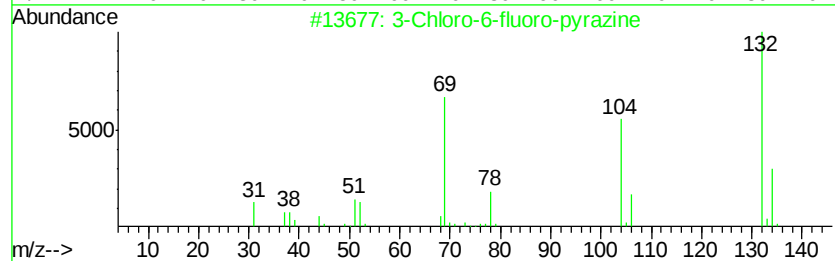
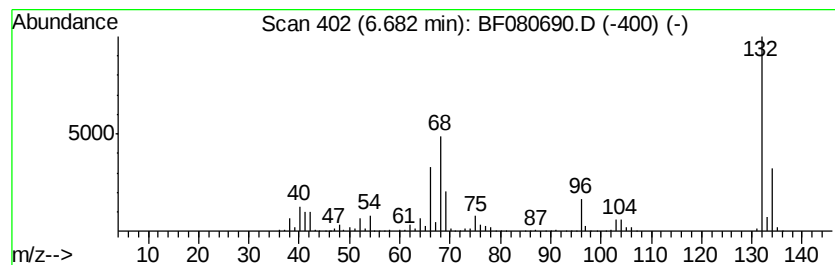
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Peak Number 4 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	125.30 ng	986772	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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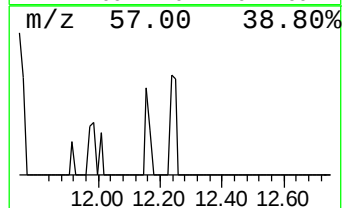
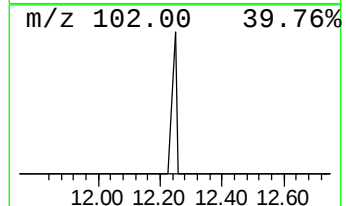
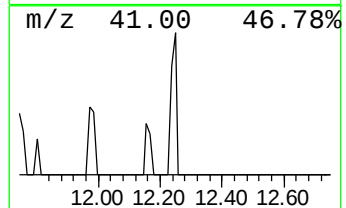
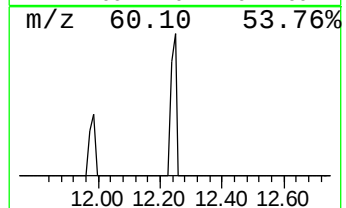
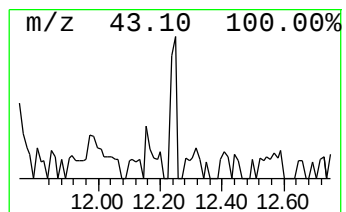
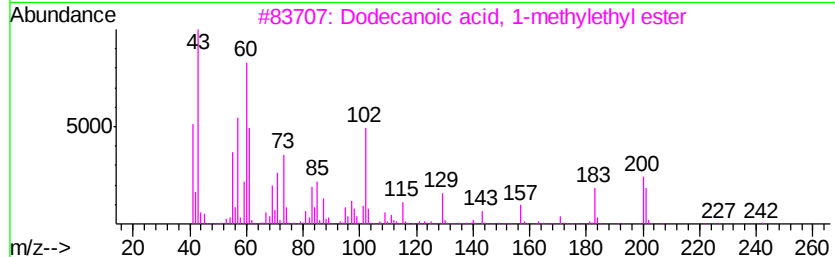
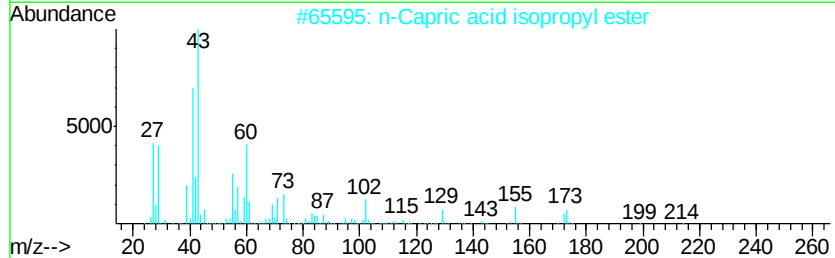
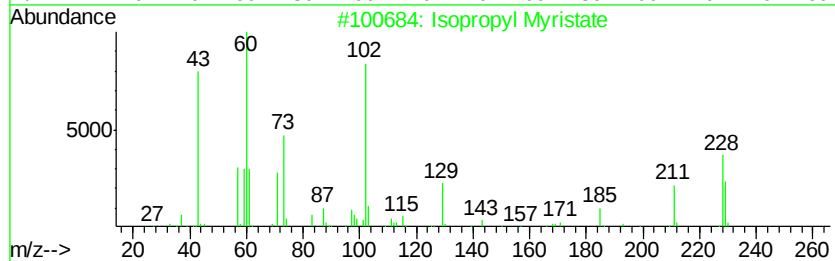
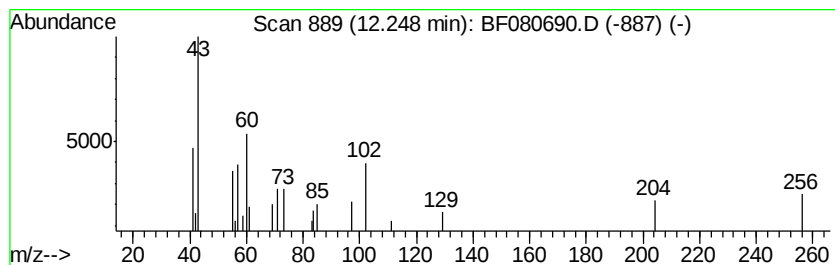
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Peak Number 6 unknown12.25 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	3.40 ng	18355	Phenanthrene-d10	11.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Myristate	270	C17H34O2	000110-27-0	38
2			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	25
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	25
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	22
5			o-Acetyl-L-serine	147	C5H9NO4	005147-00-2	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.45	2.3	ng	17812	1	6.92	157504	20.0
2-Pentanone, 4-hy...	5.09	72.3	ng	569267	1	6.92	157504	20.0
unknown6.68	6.68	125.3	ng	986772	1	6.92	157504	20.0
unknown12.25	12.25	3.4	ng	18355	4	11.45	107907	20.0