

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020817\
 Data File : BF092863.D
 Acq On : 8 Feb 2017 19:51
 Operator : SJ/MA
 Sample : I1739-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 020217-PR-E-D-M

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-BF013017.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	4.407	201	203	212	rVB	140022	222095	4.90%	0.805%
2	5.058	258	260	263	rBV	989527	1024002	22.57%	3.713%
3	5.493	295	298	300	rBV	986068	987979	21.78%	3.582%
4	5.893	331	333	336	rBV	183079	157519	3.47%	0.571%
5	6.521	386	388	395	rBV	683713	660860	14.57%	2.396%
6	6.659	398	400	402	rBV	2106249	1793787	39.54%	6.504%
7	6.887	418	420	423	rBV	638809	765872	16.88%	2.777%
8	7.047	432	434	437	rBV	2878148	2744499	60.50%	9.951%
9	7.459	467	470	472	rBV	2556580	2417088	53.28%	8.764%
10	8.179	530	533	535	rBV	1230166	1082795	23.87%	3.926%
11	9.253	624	627	630	rBV	4192110	4122188	90.87%	14.947%
12	9.928	684	686	689	rBV	1175505	1210407	26.68%	4.389%
13	10.362	720	724	726	rBV	49731	57476	1.27%	0.208%
14	10.442	728	731	733	rBV	49178	65386	1.44%	0.237%
15	10.716	753	755	758	rBV2	1312520	1548879	34.14%	5.616%
16	10.830	764	765	770	rVB	60446	72399	1.60%	0.263%
17	11.276	803	804	811	rBV	26213	47957	1.06%	0.174%
18	11.413	814	816	819	rBV	1191467	1215082	26.78%	4.406%
19	13.002	952	955	958	rBV	3364952	4536482	100.00%	16.449%
20	13.916	1031	1035	1043	rBV2	18926	51937	1.14%	0.188%
21	14.054	1044	1047	1050	rVB	1454479	1306606	28.80%	4.738%
22	15.505	1171	1174	1180	rVB	907615	1250184	27.56%	4.533%
23	15.940	1209	1212	1220	rVB	38387	71635	1.58%	0.260%
24	16.431	1252	1255	1262	rVB	34922	68435	1.51%	0.248%
25	17.003	1302	1305	1310	rVB	25607	48883	1.08%	0.177%
26	17.677	1361	1364	1370	rVB2	17964	48834	1.08%	0.177%

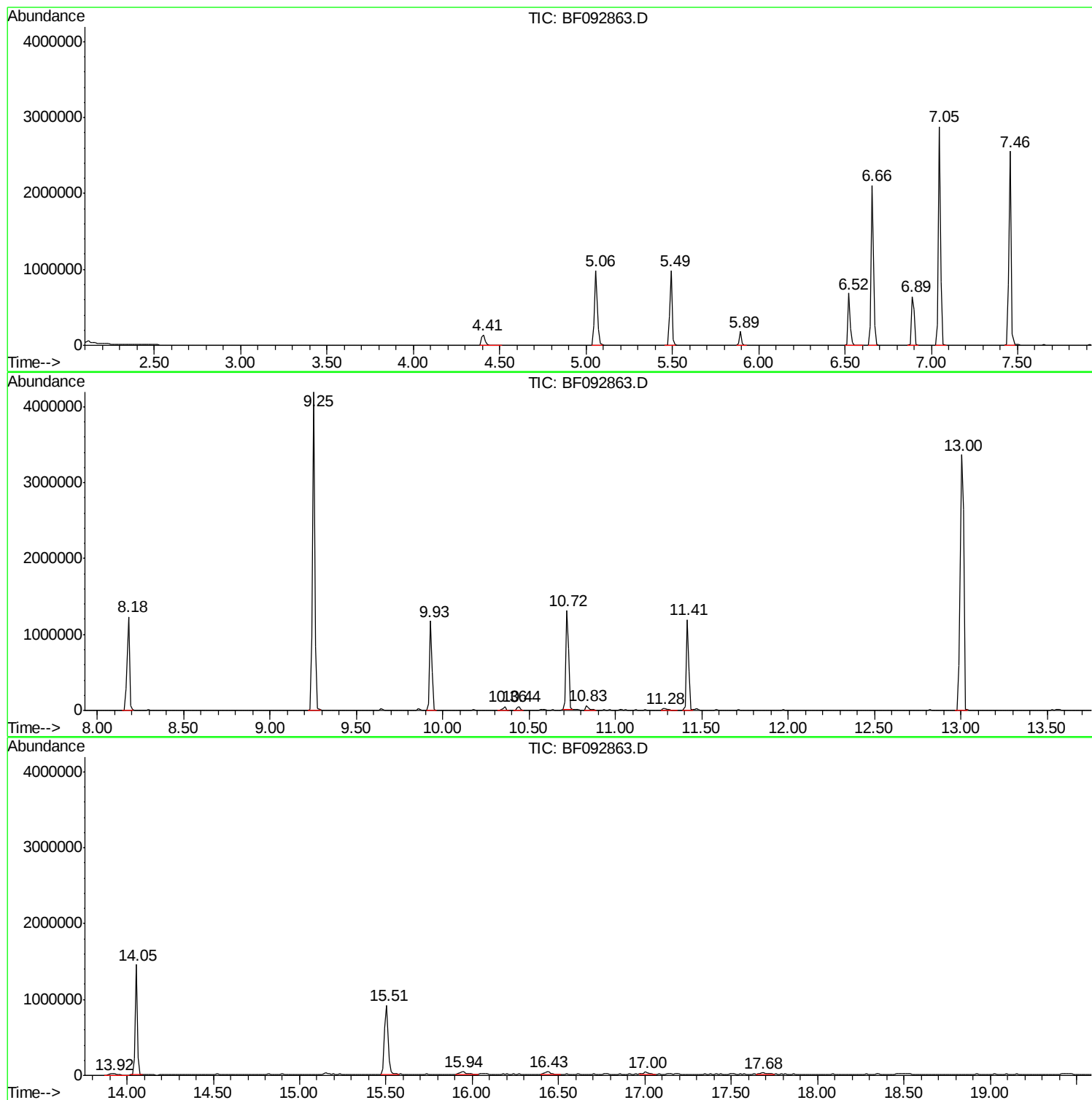
Sum of corrected areas: 27579266

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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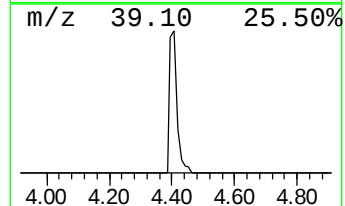
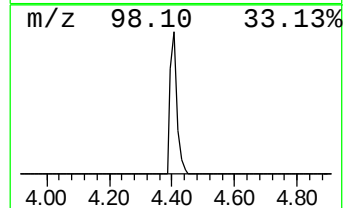
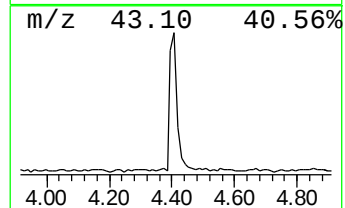
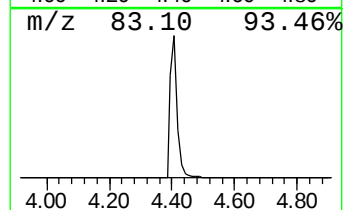
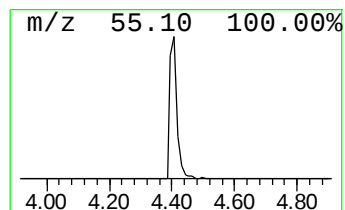
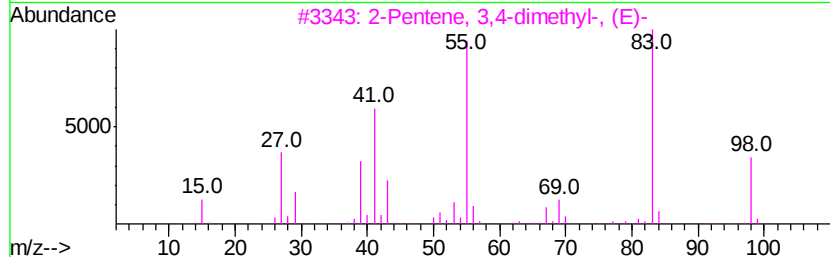
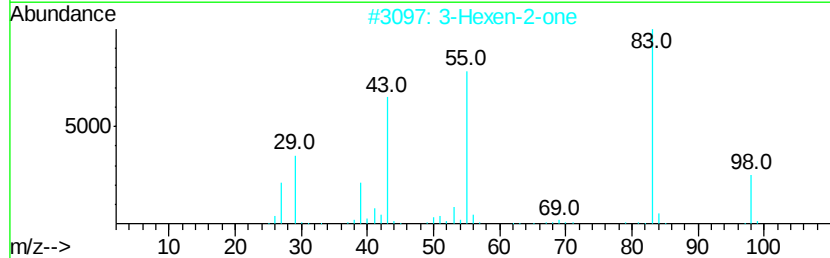
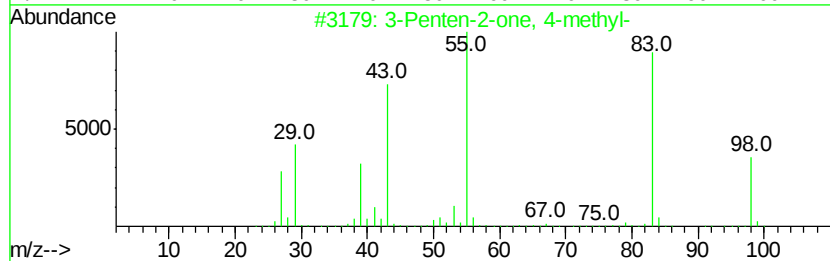
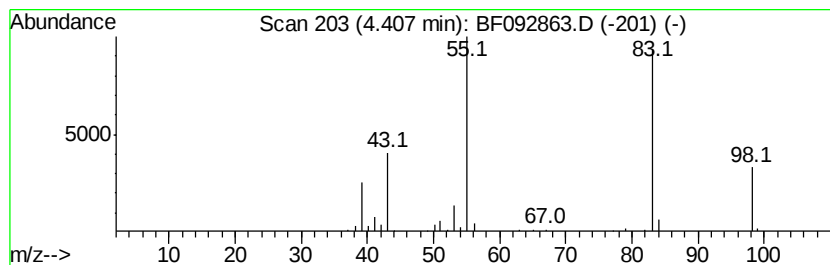
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	5.80 ng	222095	1,4-Dichlorobenzene-d4	6.89

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	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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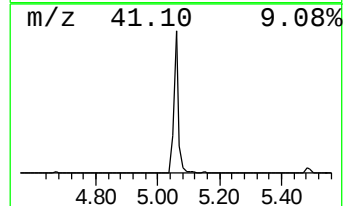
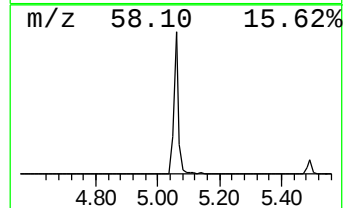
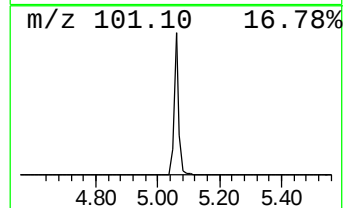
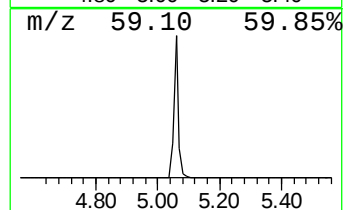
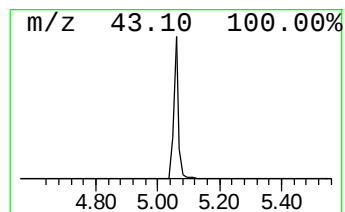
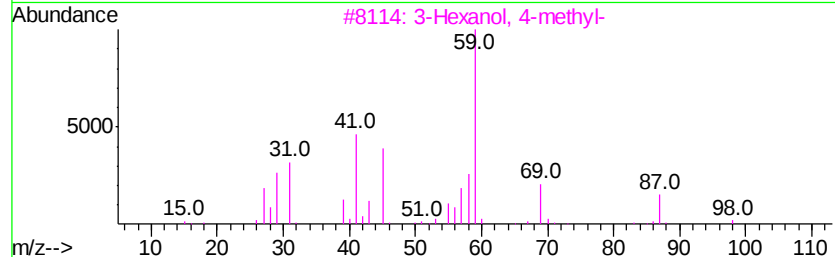
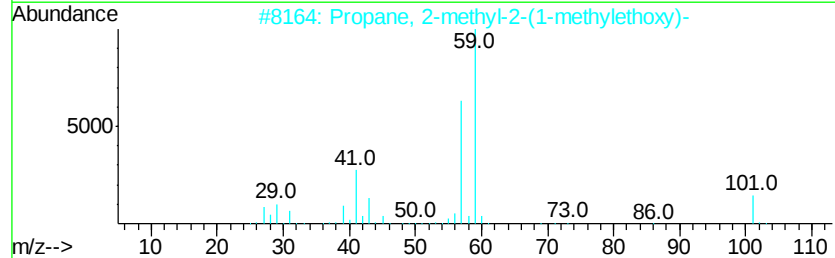
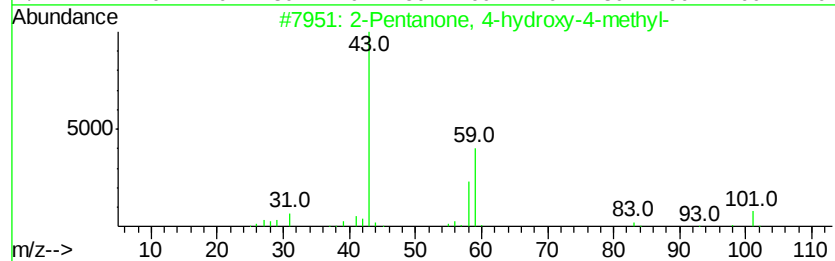
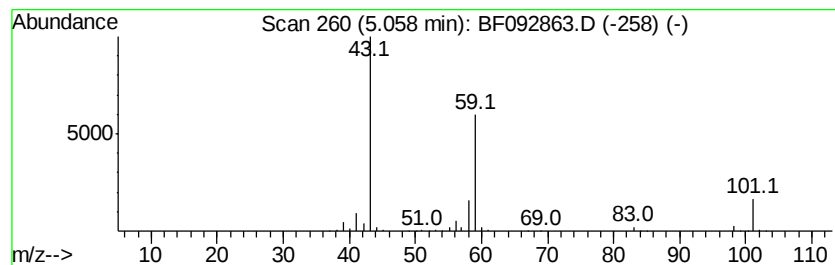
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
5.06	26.74 ng	1024000	1,4-Dichlorobenzene-d4	6.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32	



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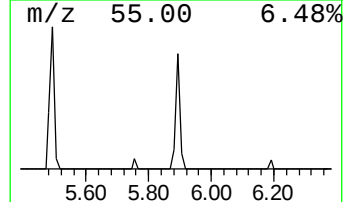
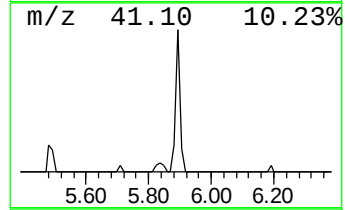
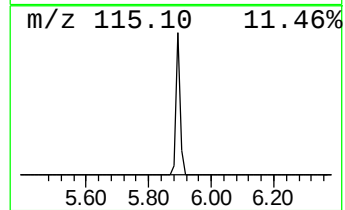
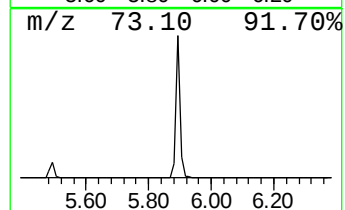
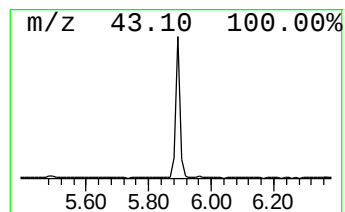
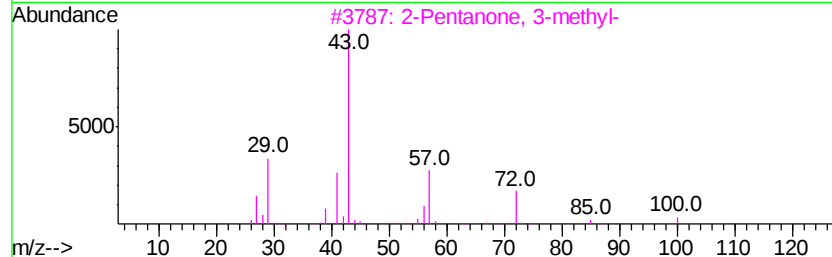
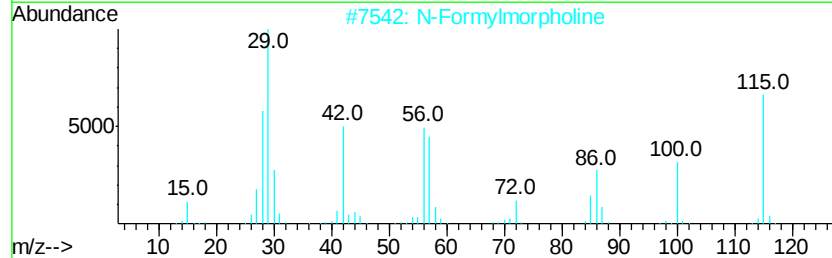
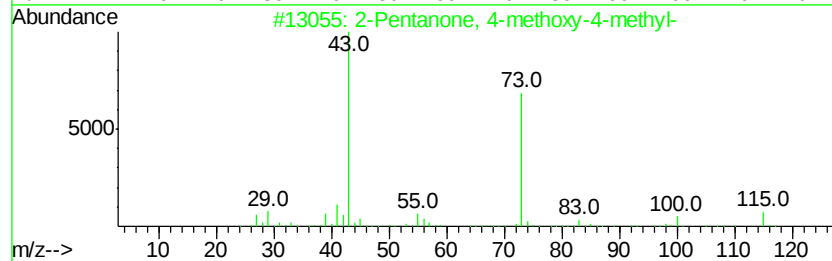
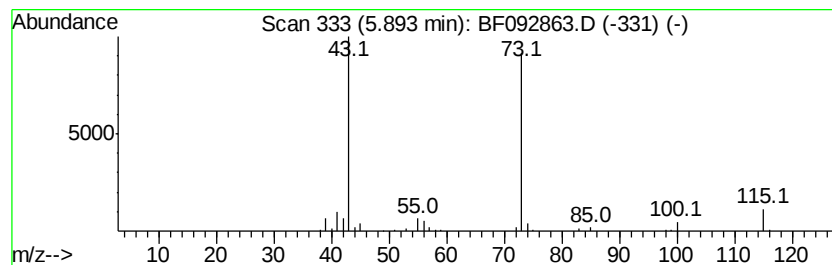
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.11 ng	157519	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	9



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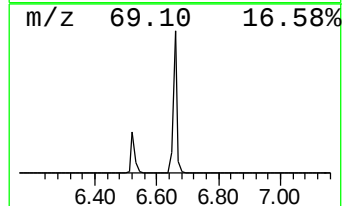
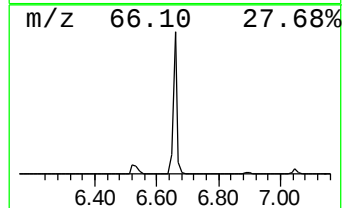
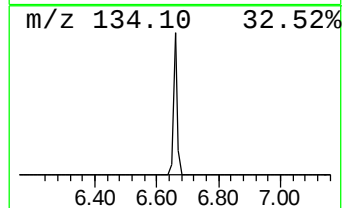
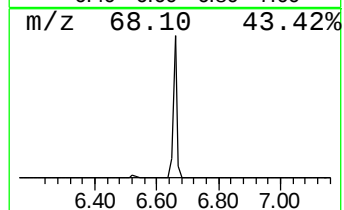
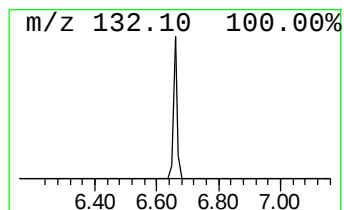
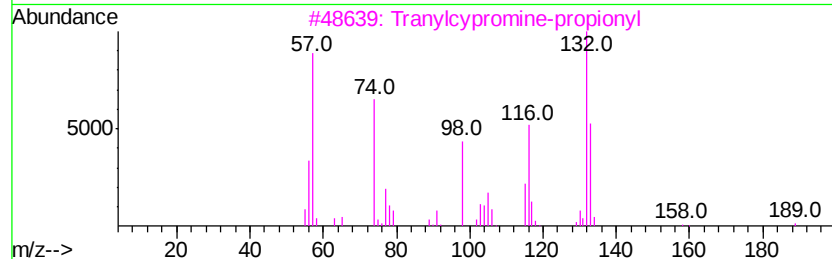
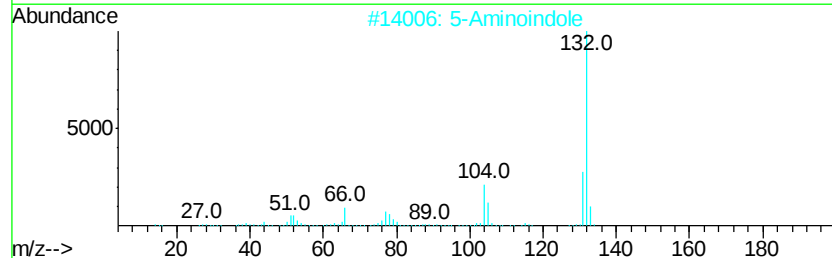
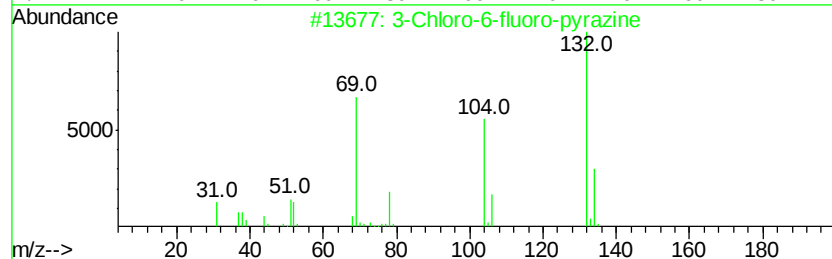
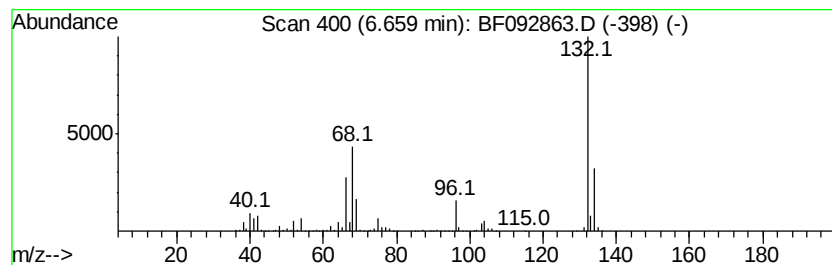
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Peak Number 4 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	46.84 ng	1793790	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.41	5.8	ng	222095	1	6.89	765872	20.0
2-Pentanone, 4-hy...	5.06	26.7	ng	1024000	1	6.89	765872	20.0
2-Pentanone, 4-me...	5.89	4.1	ng	157519	1	6.89	765872	20.0
unknown6.66	6.66	46.8	ng	1793790	1	6.89	765872	20.0