

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051816\
 Data File : BF087167.D
 Acq On : 19 May 2016 3:21
 Operator : UM/SJ
 Sample : PB90659BL
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90659BL

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-BF051716.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	1.713	10	11	57	rVB	3587559	7305370	100.00%	18.580%
2	3.964	206	208	219	rBV	74416	149650	2.05%	0.381%
3	4.707	270	273	288	rBV	1033338	1922528	26.32%	4.890%
4	5.164	311	313	330	rBV	2506153	3396257	46.49%	8.638%
5	5.564	347	348	356	rVB	117133	143485	1.96%	0.365%
6	6.239	405	407	410	rBV	2415567	3221781	44.10%	8.194%
7	6.353	414	417	419	rBV	2912990	3511193	48.06%	8.930%
8	6.570	434	436	439	rBV	562511	779998	10.68%	1.984%
9	6.730	447	450	453	rBV	2839640	2583862	35.37%	6.572%
10	7.153	484	487	489	rBV	2354947	2408619	32.97%	6.126%
11	7.862	547	549	552	rBV	1055253	1006605	13.78%	2.560%
12	8.948	641	644	646	rBV	3392432	3802264	52.05%	9.671%
13	9.610	699	702	704	rBV	1191912	1077706	14.75%	2.741%
14	10.399	768	771	788	rBV	2158051	2208559	30.23%	5.617%
15	11.085	829	831	834	rBV	1120276	995544	13.63%	2.532%
16	12.674	967	970	972	rBV	2907881	3250096	44.49%	8.266%
17	13.714	1058	1061	1063	rBV	725179	779449	10.67%	1.982%
18	15.062	1176	1179	1187	rBV	691170	774939	10.61%	1.971%

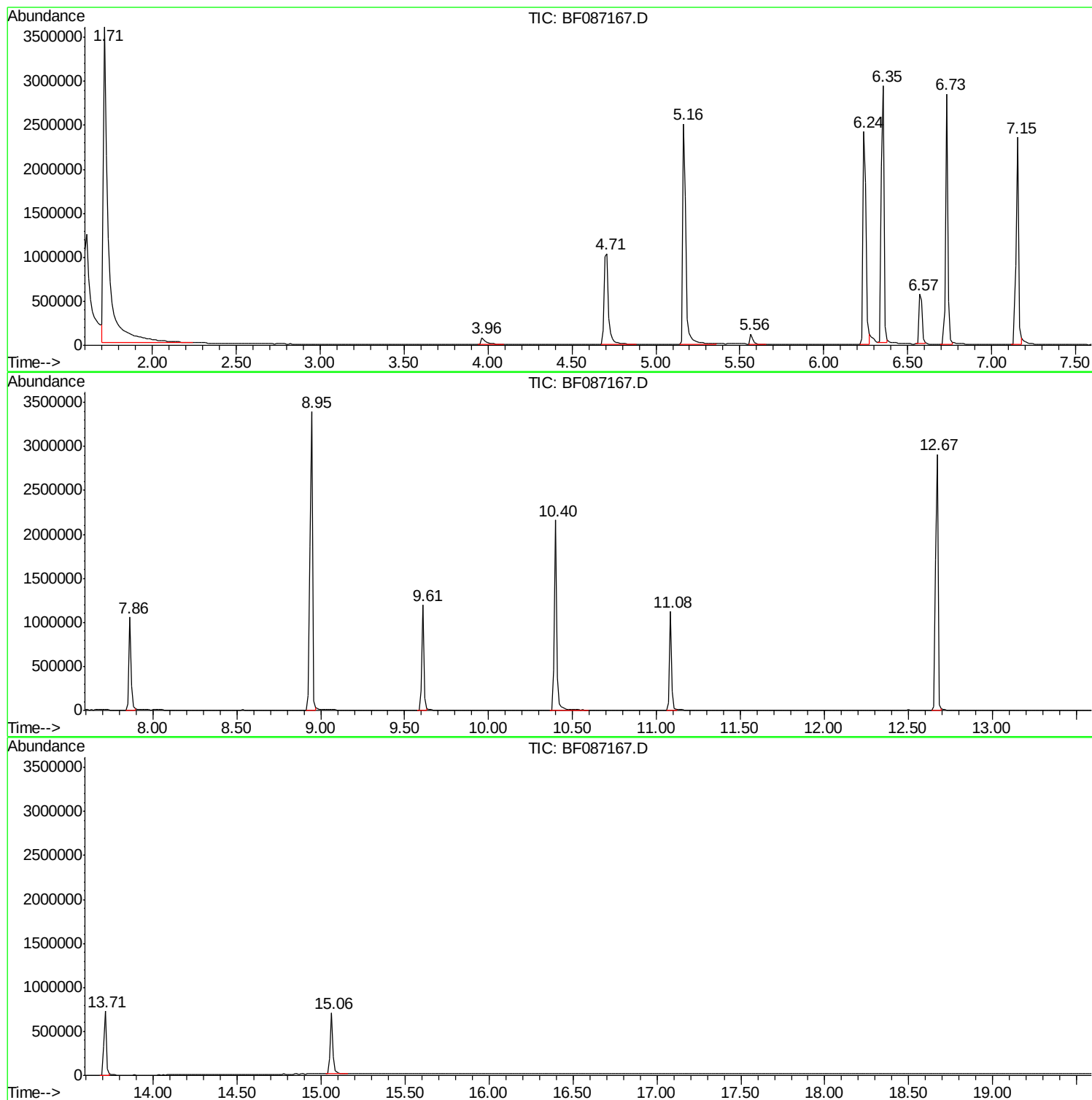
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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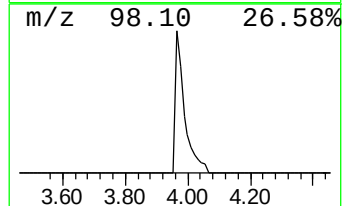
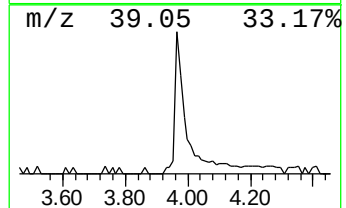
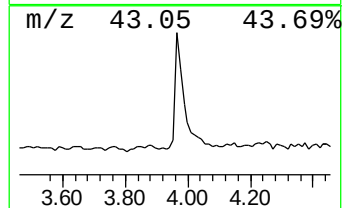
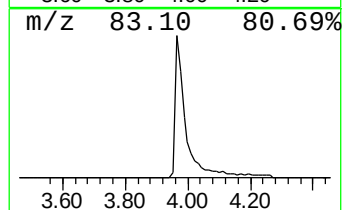
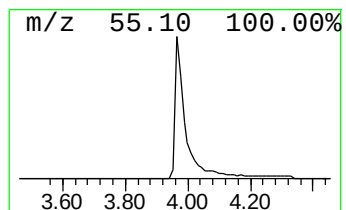
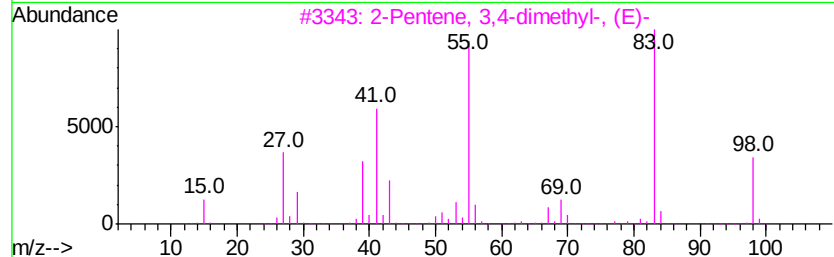
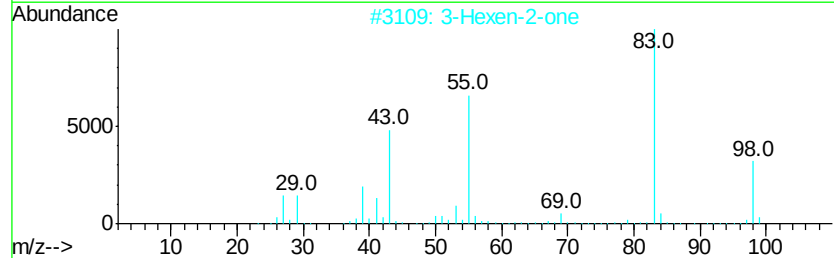
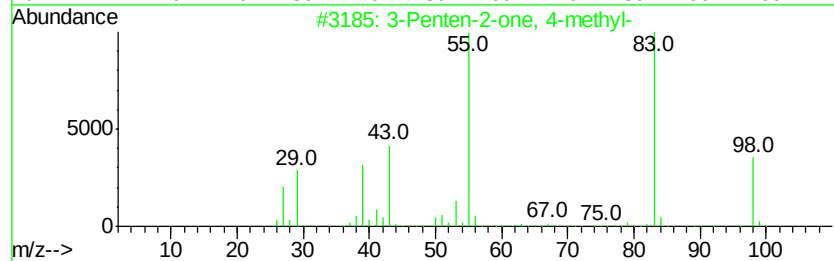
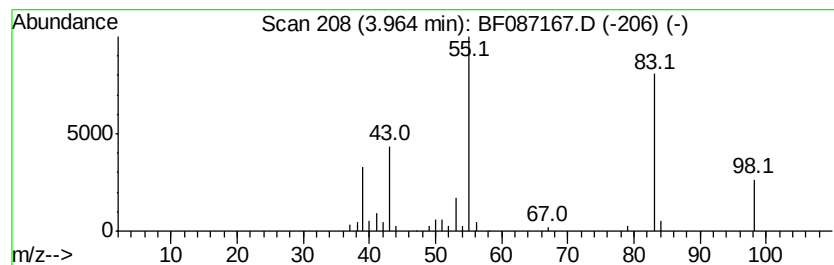
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.96	3.84 ng	149650	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
5		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	72



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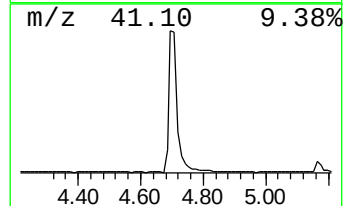
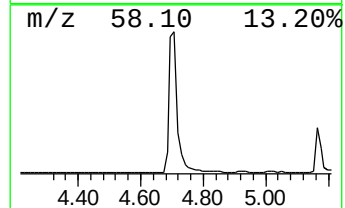
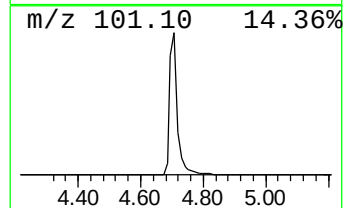
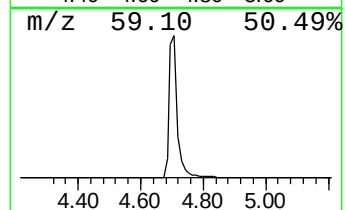
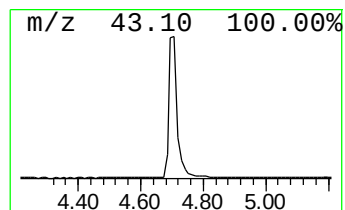
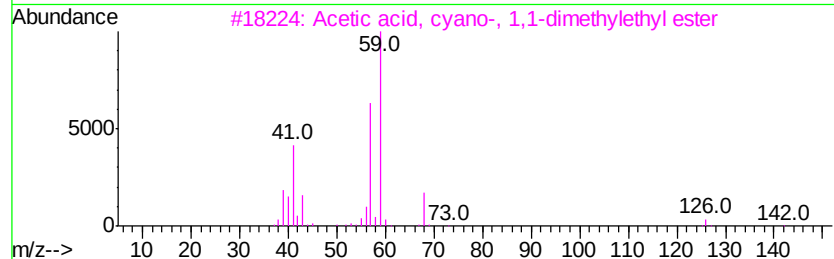
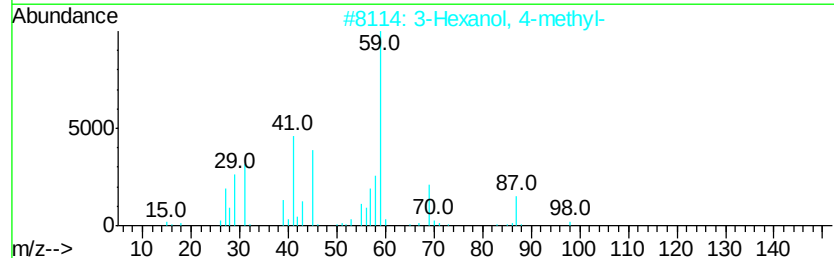
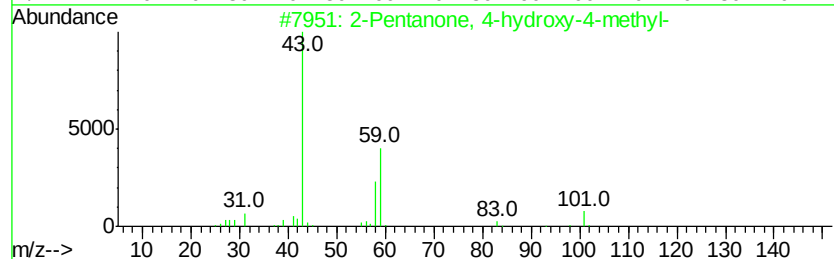
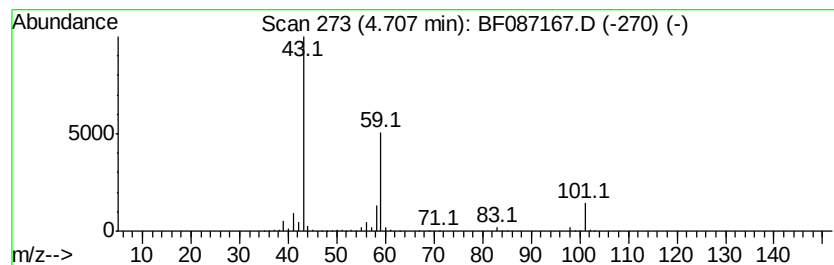
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	49.30 ng	1922530	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
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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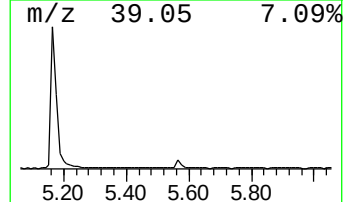
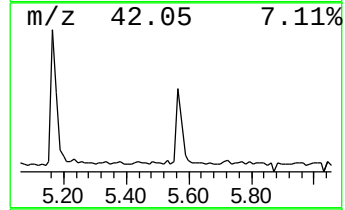
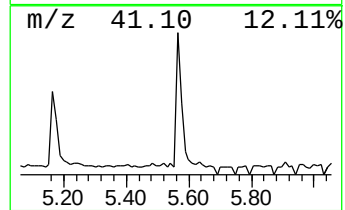
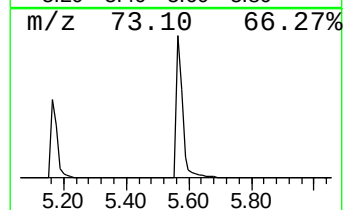
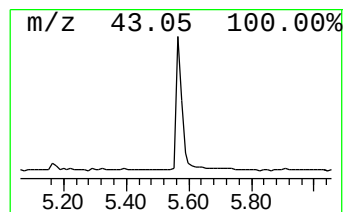
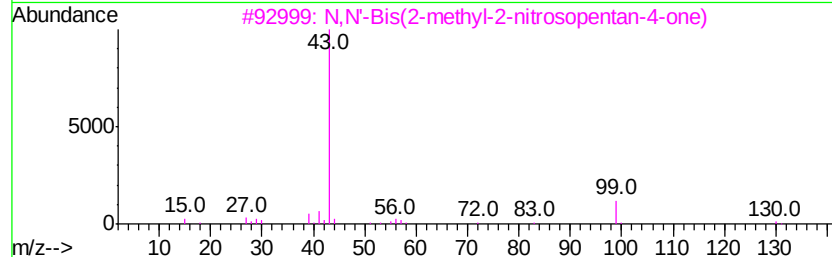
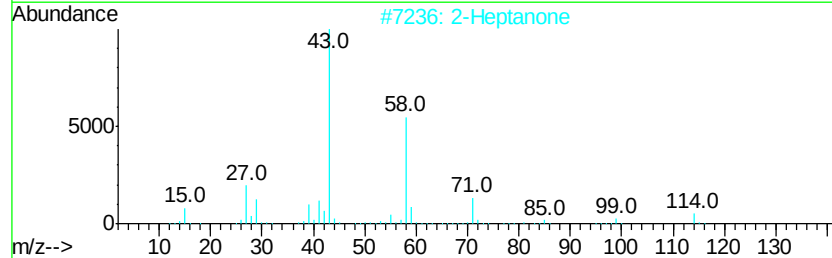
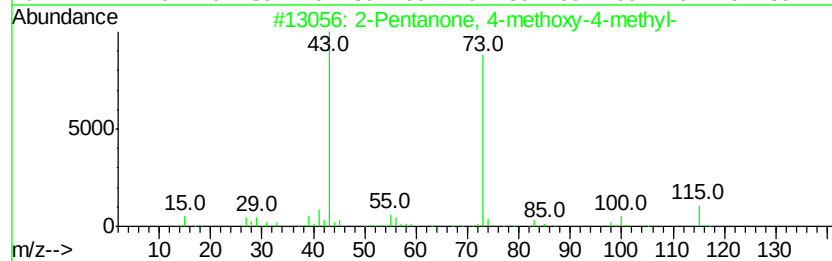
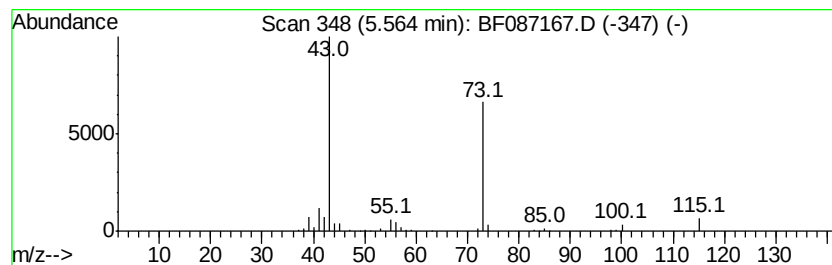
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.56	3.68 ng	143485	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		2-Heptanone	114	C7H14O	000110-43-0	23
3		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	23
4		1,3-Dioxolane, 2-ethenyl-	100	C5H8O2	003984-22-3	16
5		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	16



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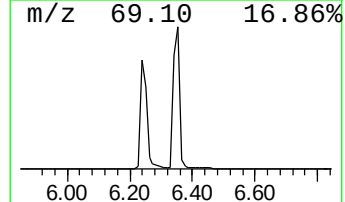
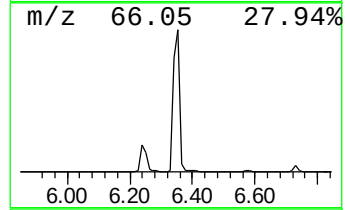
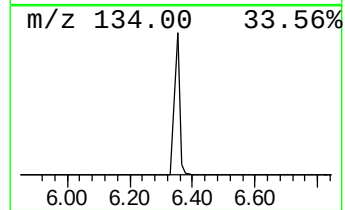
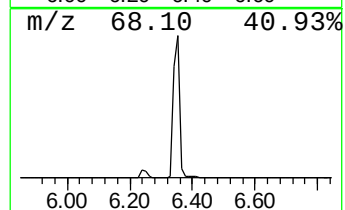
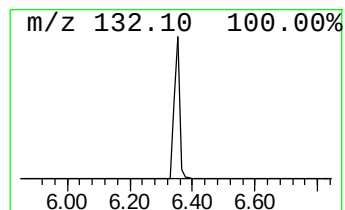
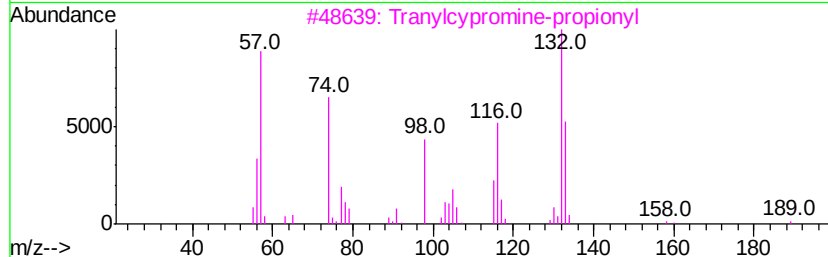
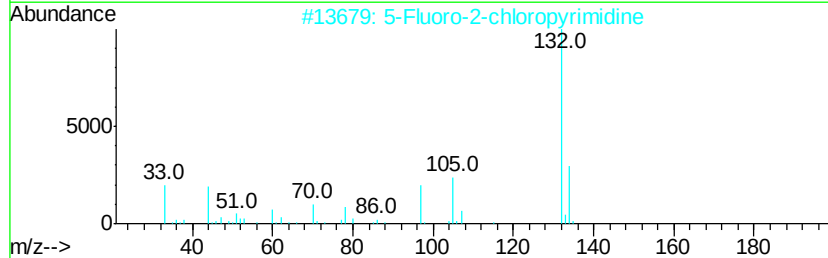
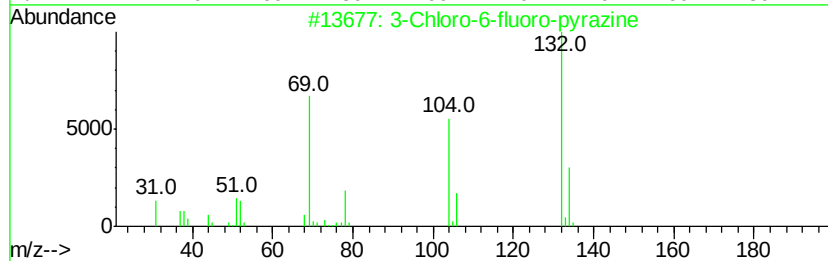
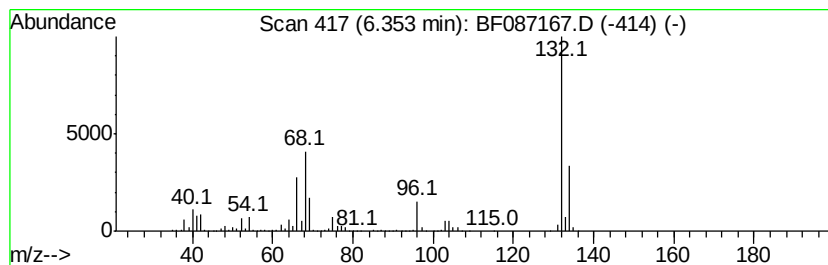
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Peak Number 5 unknown6.35 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	90.03 ng	3511190	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	Tranvlcvpromine-propionyl			189	C12H15NO	1000123-86-3	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE			132	C8H8N2	1000241-93-9	10
5	Benzene, 1,2,4-trifluoro-			132	C6H3F3	000367-23-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.96	3.8	ng	149650	1	6.58	779998	20.0
2-Pentanone, 4-hy...	4.71	49.3	ng	1922530	1	6.58	779998	20.0
2-Pentanone, 4-me...	5.56	3.7	ng	143485	1	6.58	779998	20.0
unknown6.35	6.35	90.0	ng	3511190	1	6.58	779998	20.0