

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
 Data File : BF094283.D
 Acq On : 7 Apr 2017 20:03
 Operator : SJ/MA
 Sample : I2534-08
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GP-B-03(5-10)

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-BF032217.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	3.451	262	266	277	rVB	138270	163131	3.62%	0.445%
2	4.010	356	361	369	rVB	756660	943726	20.93%	2.573%
3	4.439	429	434	437	rBV	4085244	4136600	91.76%	11.277%
4	5.528	612	619	622	rBV	3401460	4273243	94.79%	11.649%
5	5.628	631	636	639	rBV	4151985	4329670	96.04%	11.803%
6	5.857	671	675	679	rBV	1040119	917964	20.36%	2.502%
7	6.039	701	706	709	rBV	3400225	3377900	74.93%	9.208%
8	6.510	780	786	789	rBV	2280901	2854762	63.32%	7.782%
9	6.722	816	822	825	rBV	54307	58174	1.29%	0.159%
10	7.057	875	879	882	rBV2	61203	56290	1.25%	0.153%
11	7.363	924	931	934	rBV	1229961	1240348	27.51%	3.381%
12	8.127	1057	1061	1064	rBV	181132	160507	3.56%	0.438%
13	8.686	1149	1156	1159	rBV	4214658	4508161	100.00%	12.290%
14	9.022	1209	1213	1221	rBV	32507	56479	1.25%	0.154%
15	9.180	1236	1240	1244	rBV	406253	353591	7.84%	0.964%
16	9.504	1291	1295	1300	rVB2	1158469	1223947	27.15%	3.337%
17	10.092	1391	1395	1399	rVB	83049	80724	1.79%	0.220%
18	10.486	1455	1462	1465	rBV	2088925	2275663	50.48%	6.204%
19	10.674	1491	1494	1496	rBV	95529	98471	2.18%	0.268%
20	11.227	1585	1588	1592	rBV	64487	68014	1.51%	0.185%
21	11.327	1600	1605	1609	rBV	1060263	1034149	22.94%	2.819%
22	12.063	1726	1730	1737	rBV2	140013	200028	4.44%	0.545%
23	13.309	1936	1942	1945	rBV	2317755	2718318	60.30%	7.410%
24	14.580	2154	2158	2171	rVB	883627	1552923	34.45%	4.233%

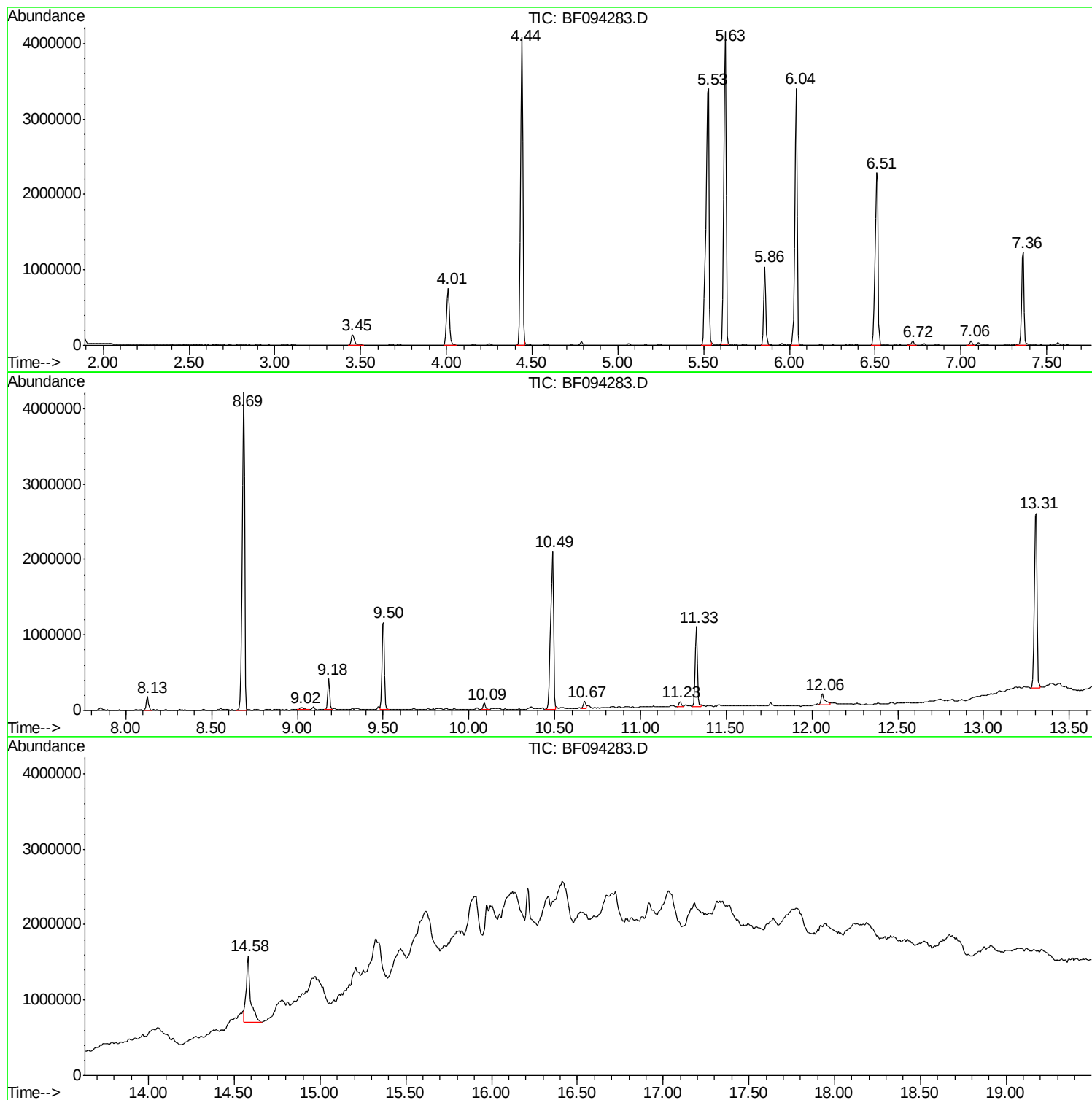
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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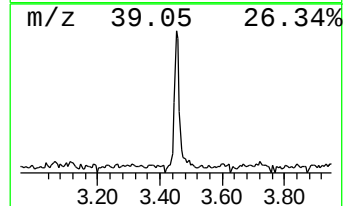
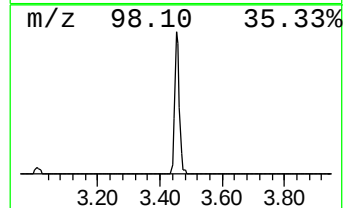
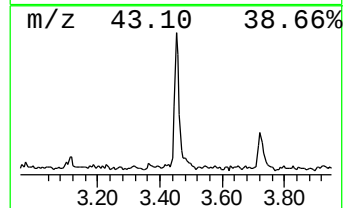
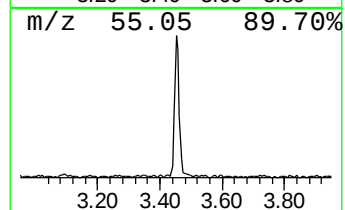
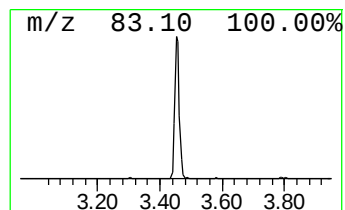
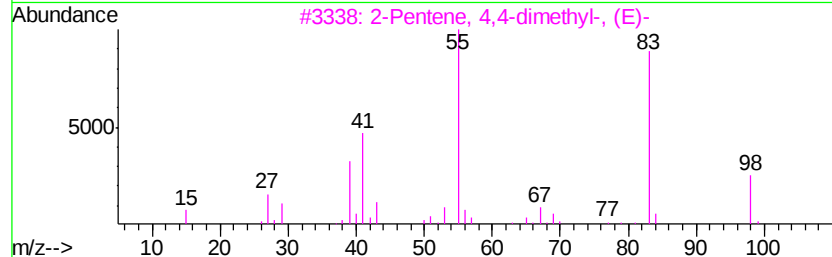
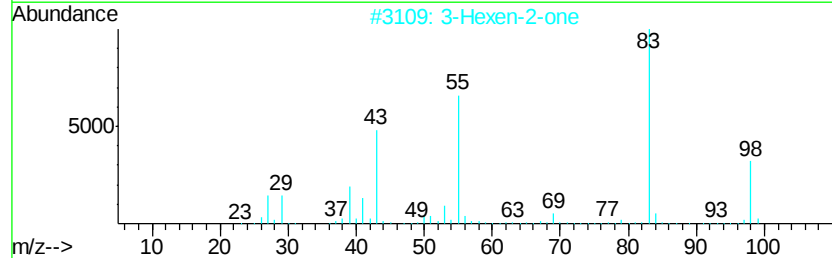
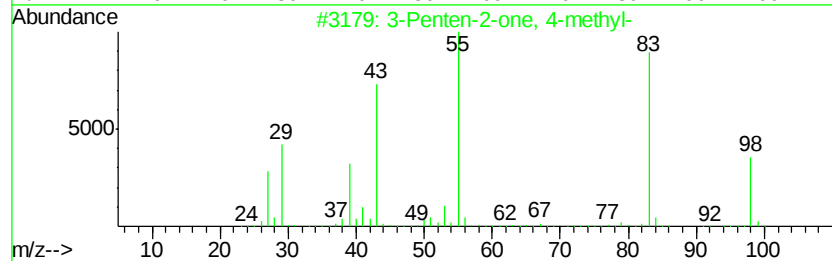
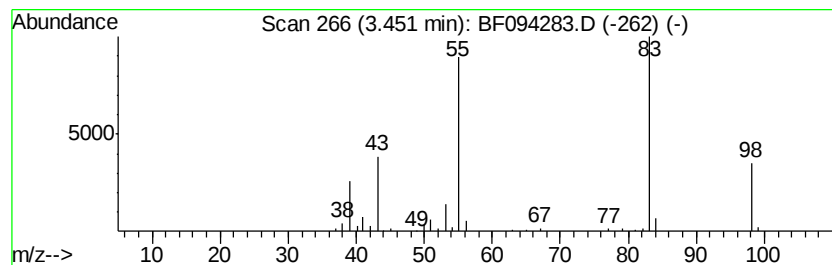
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.45	3.55 ng	163131	1,4-Dichlorobenzene-d4	5.86

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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83



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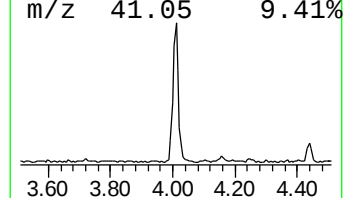
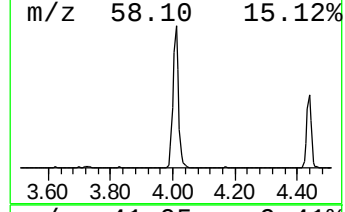
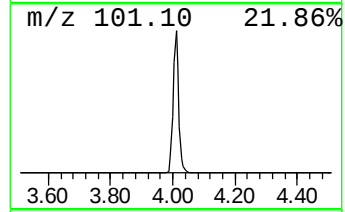
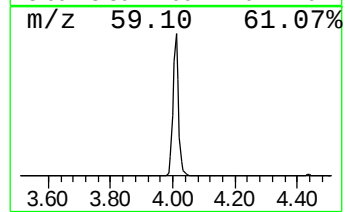
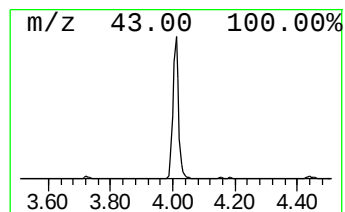
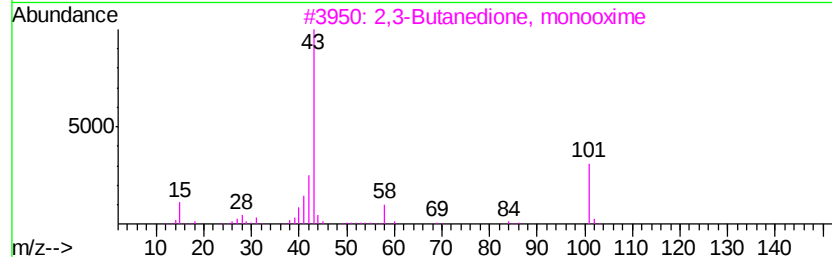
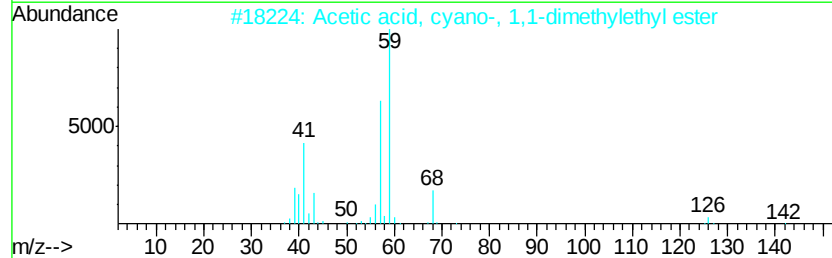
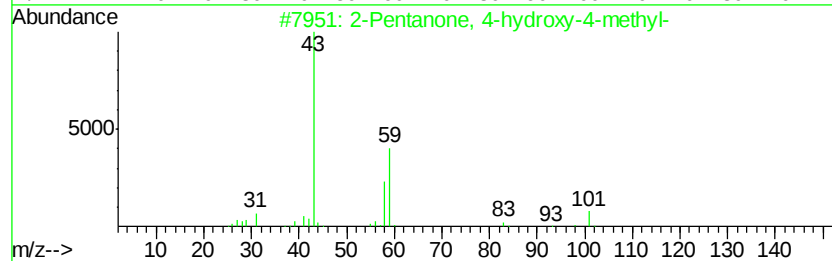
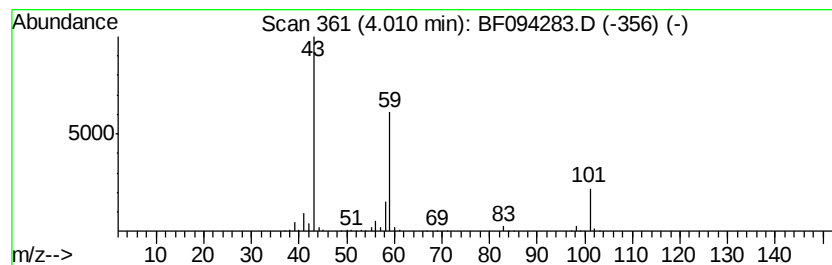
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	20.56 ng	943726	1,4-Dichlorobenzene-d4	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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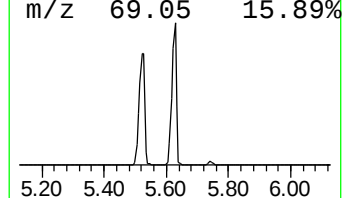
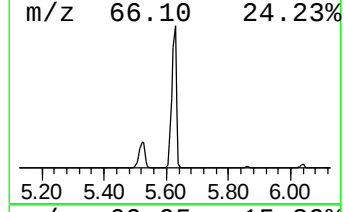
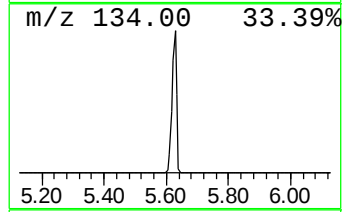
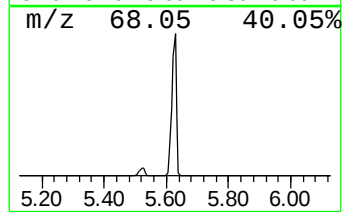
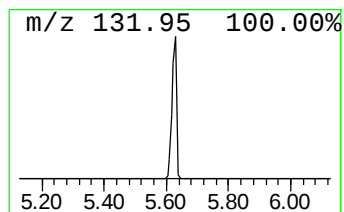
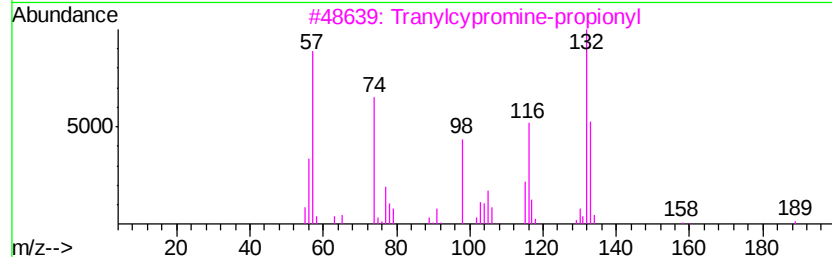
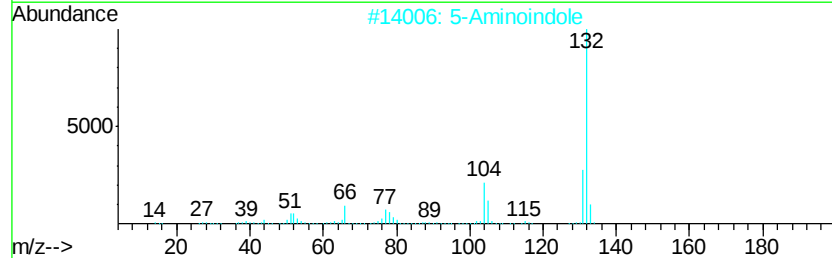
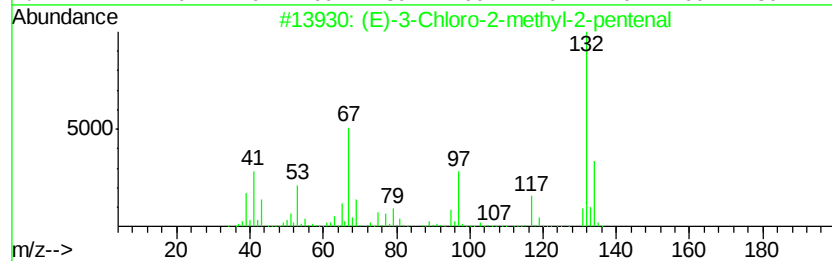
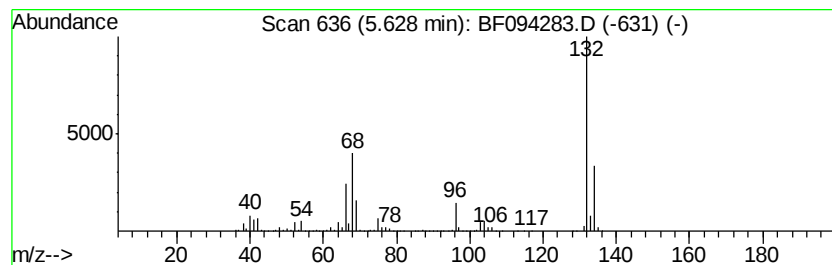
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	94.33 ng	4329670	1,4-Dichlorobenzene-d4	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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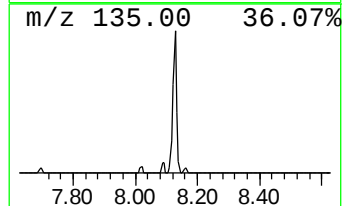
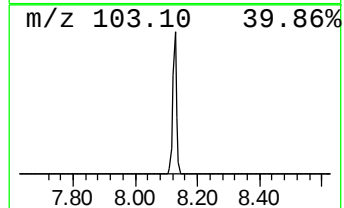
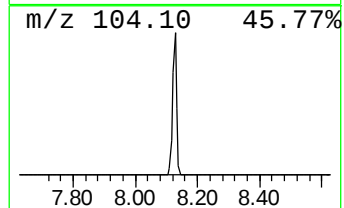
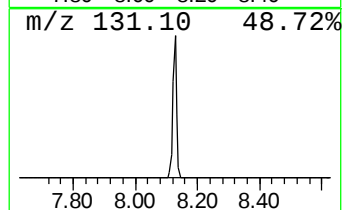
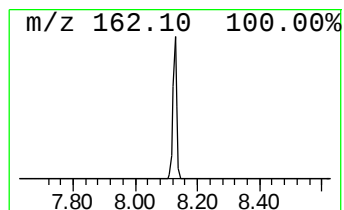
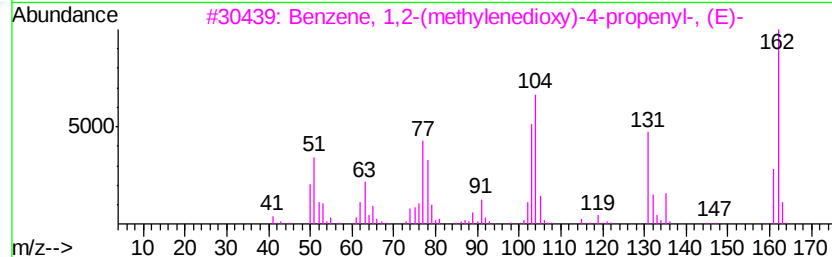
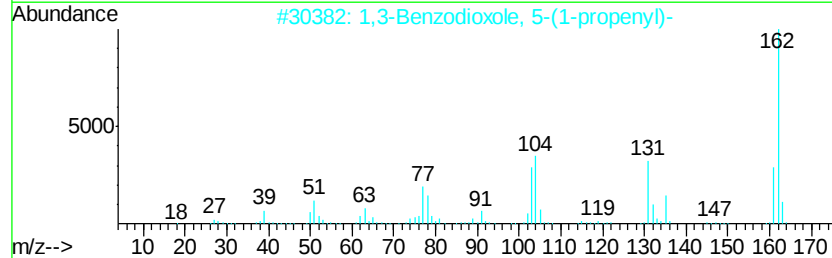
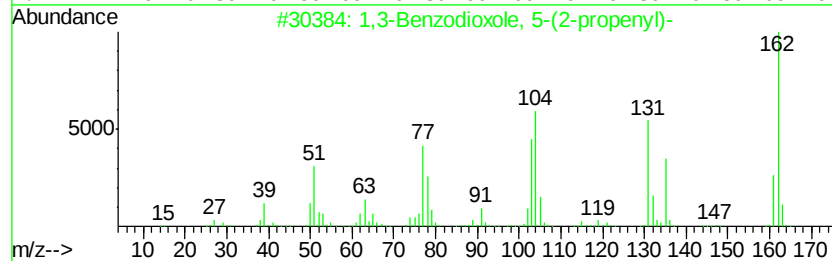
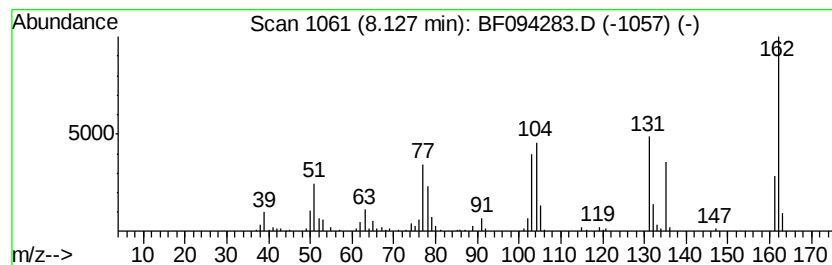
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Peak Number 5 1,3-Benzodioxole, 5-(2-prop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	2.59 ng	160507	Napthalene-d8	7.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzodioxole, 5-(2-propenyl)-	162	C10H10O2	000094-59-7	98
2			1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3			Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	93
4			1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	90
5			1,4-Dioxo-1,2,3,4-tetrahydrophth...	162	C8H6N2O2	001445-69-8	38



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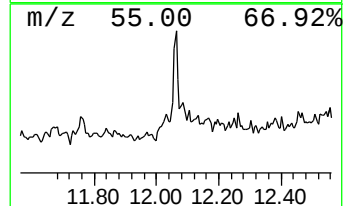
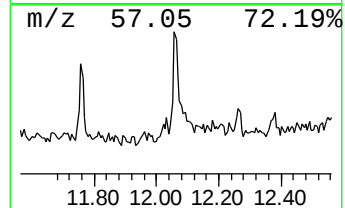
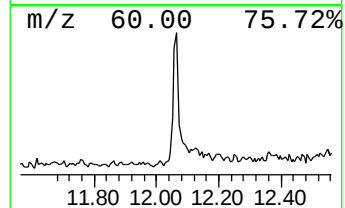
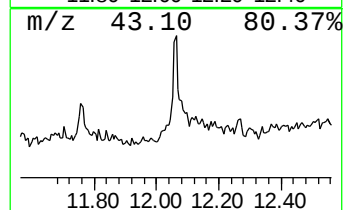
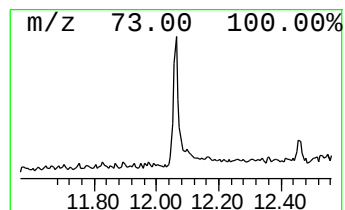
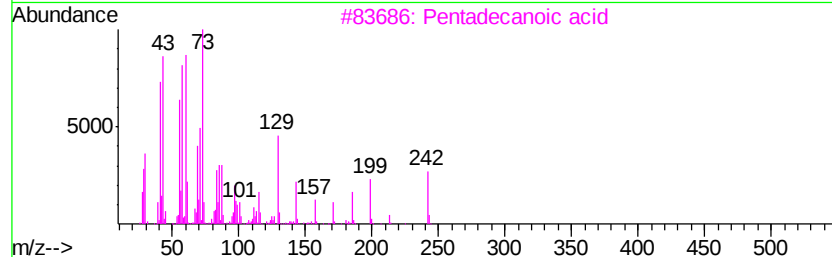
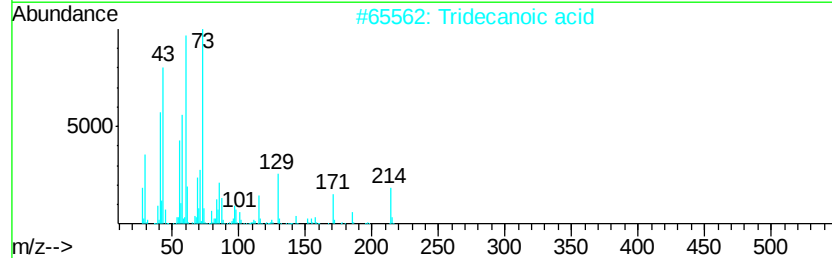
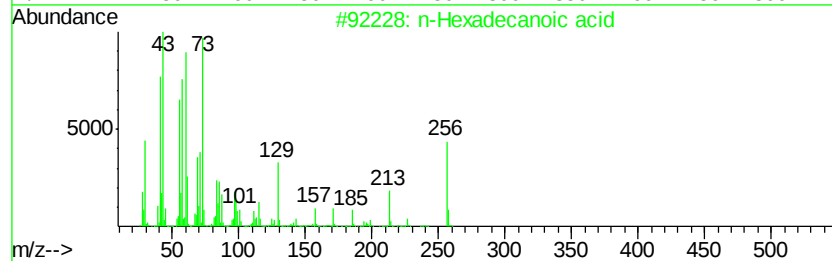
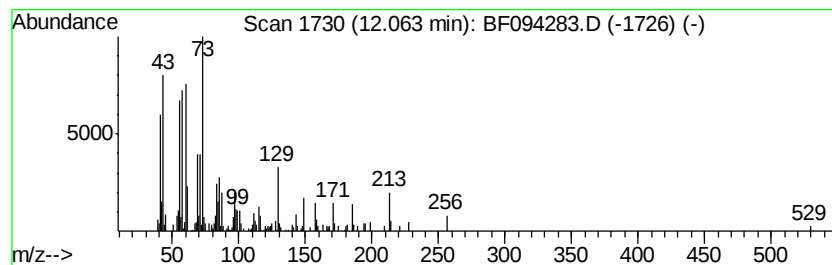
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	3.87 ng	200028	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	70



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.45	3.5	ng	163131	1	5.86	917964	20.0
2-Pentanone, 4-hy...	4.01	20.6	ng	943726	1	5.86	917964	20.0
unknown5.63	5.63	94.3	ng	4329670	1	5.86	917964	20.0
1,3-Benzodioxole,...	8.13	2.6	ng	160507	2	7.36	1240350	20.0
n-Hexadecanoic acid	12.06	3.9	ng	200028	4	11.33	1034150	20.0