

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
 Data File : BF088535.D
 Acq On : 30 Jun 2016 18:04
 Operator : UM/SJ
 Sample : PB91573BL
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91573BL

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-BF063016.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	1.735	12	13	23	rVV	731210	1097270	27.19%	2.587%
2	1.872	23	25	76	rVB	1604380	4036090	100.00%	9.515%
3	4.341	238	241	244	rBV	936545	1231190	30.50%	2.902%
4	5.004	295	299	305	rVB	1060091	1511254	37.44%	3.563%
5	5.416	332	335	338	rBV	2745922	3574957	88.57%	8.428%
6	6.444	421	425	427	rBV	2969052	3329689	82.50%	7.850%
7	6.581	434	437	439	rBV	3408615	3557751	88.15%	8.387%
8	6.810	455	457	459	rBV	1014055	922373	22.85%	2.174%
9	6.970	468	471	473	rVB	3031986	2815511	69.76%	6.637%
10	7.382	503	507	509	rBV	1700556	2644822	65.53%	6.235%
11	8.102	567	570	572	rBV	913577	1277903	31.66%	3.013%
12	9.176	660	664	666	rBV	3852048	4034559	99.96%	9.511%
13	9.850	720	723	725	rBV	1356568	1459411	36.16%	3.440%
14	10.628	788	791	794	rBV2	1791461	2509012	62.16%	5.915%
15	11.325	849	852	854	rBV	1769805	1500244	37.17%	3.537%
16	12.742	974	976	979	rVB	279216	258979	6.42%	0.611%
17	12.822	979	983	985	rVB	59280	60306	1.49%	0.142%
18	12.914	988	991	994	rBV	3629140	3862862	95.71%	9.106%
19	13.451	1035	1038	1040	rBV	182437	159577	3.95%	0.376%
20	13.496	1040	1042	1046	rVB	33355	50414	1.25%	0.119%
21	13.954	1079	1082	1084	rBV	1308793	1429571	35.42%	3.370%
22	15.348	1201	1204	1207	rBV	819098	1054087	26.12%	2.485%
23	15.417	1207	1210	1213	rVB	24538	40968	1.02%	0.097%

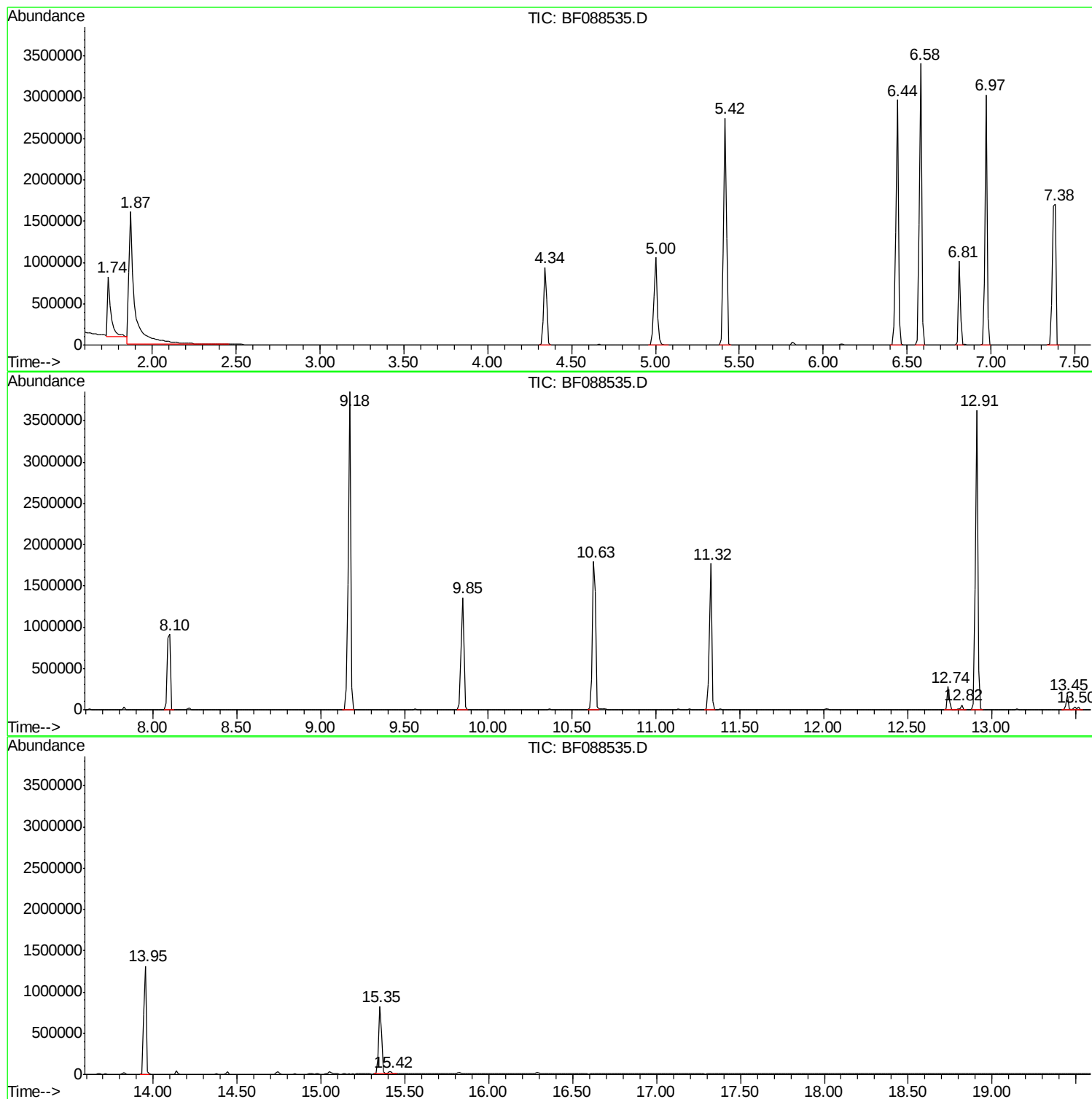
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ClientSampled :
PB91573BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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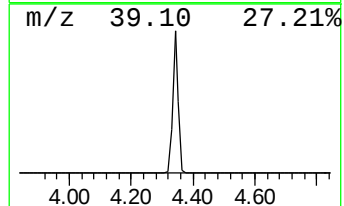
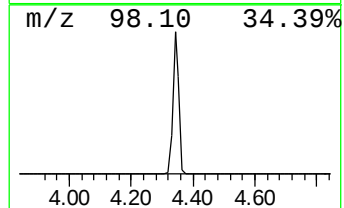
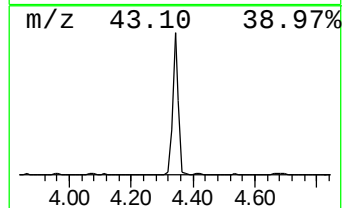
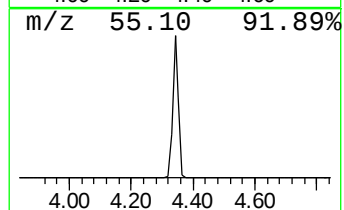
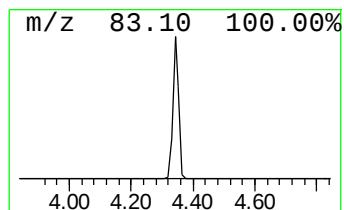
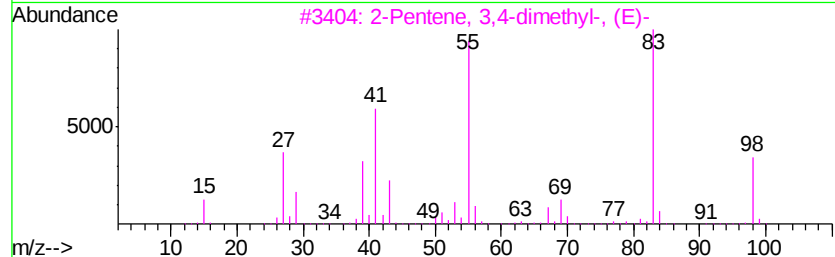
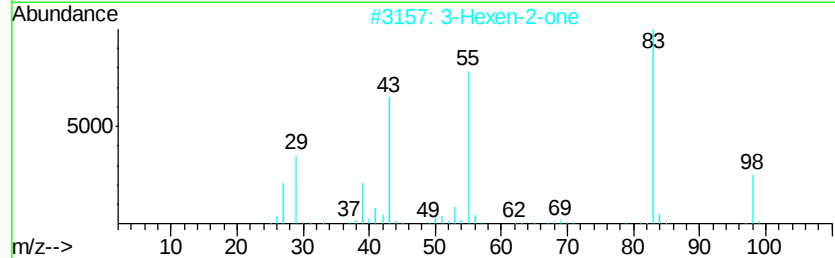
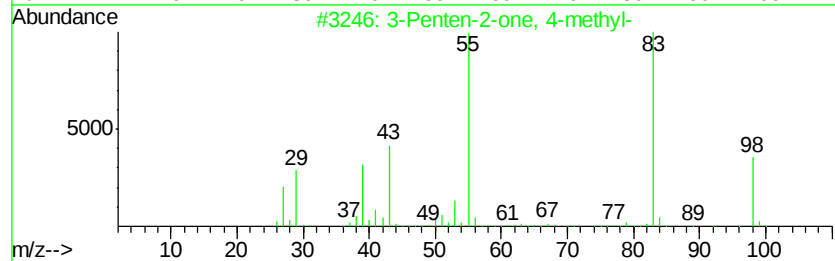
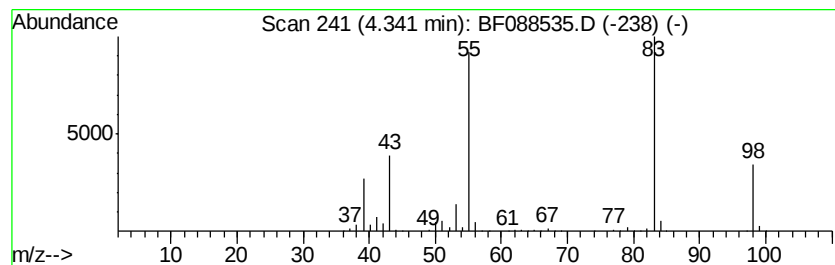
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.34	26.70 ng	1231190	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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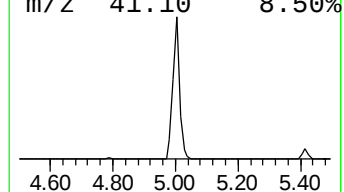
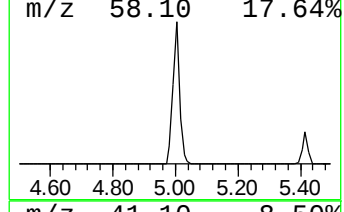
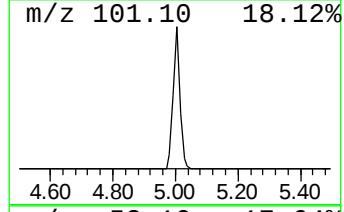
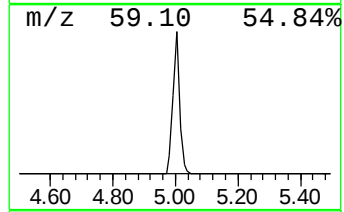
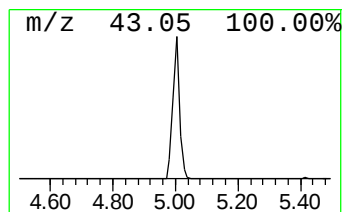
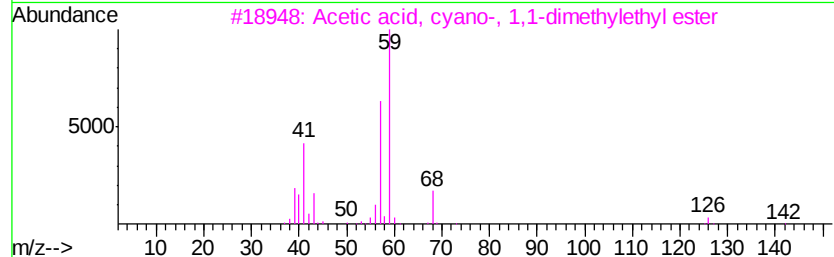
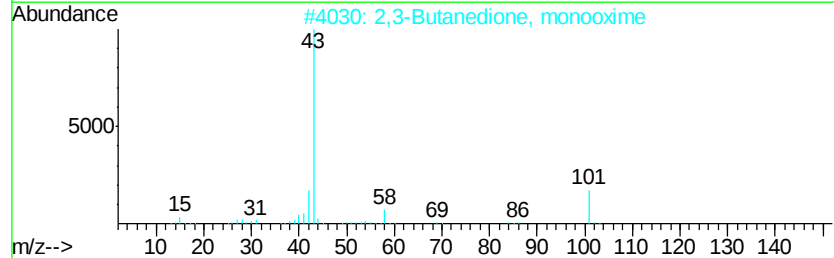
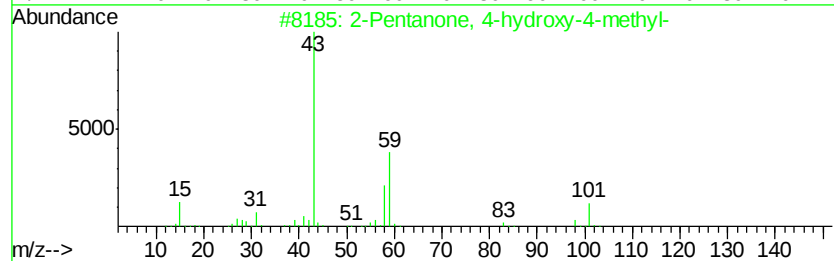
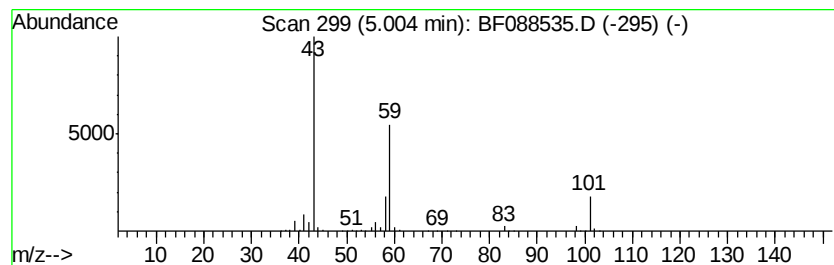
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	32.77 ng	1511250	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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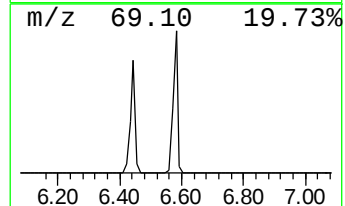
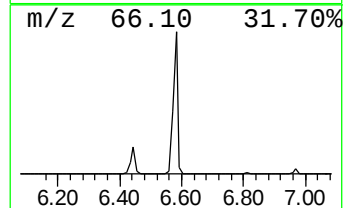
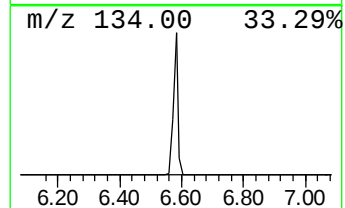
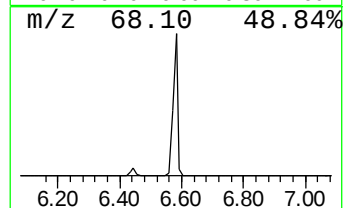
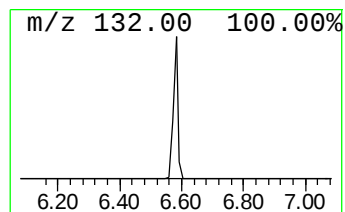
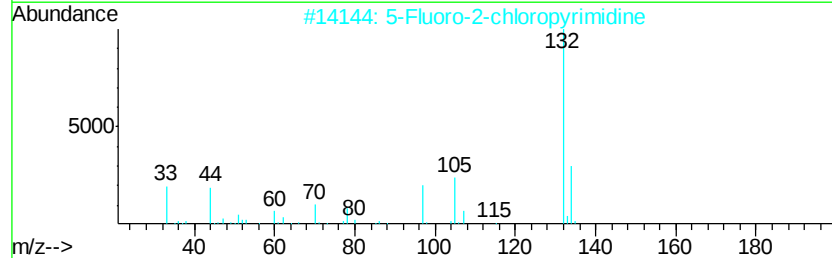
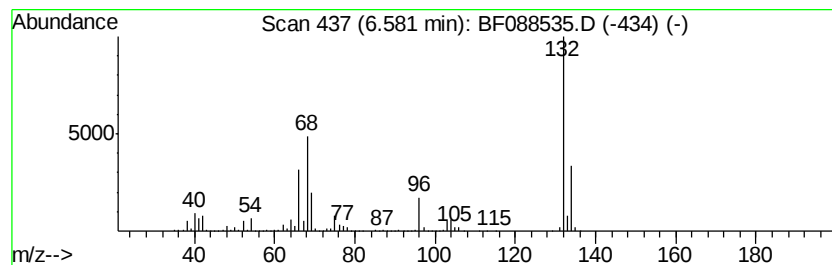
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Peak Number 5 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	77.14 ng	3557750	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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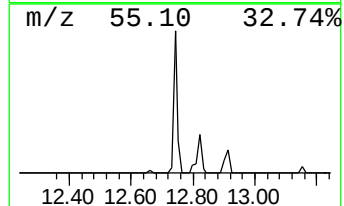
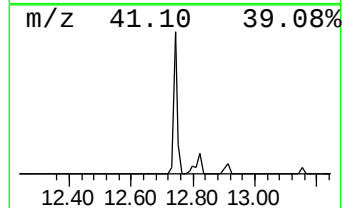
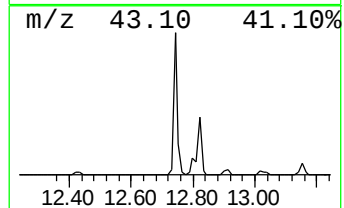
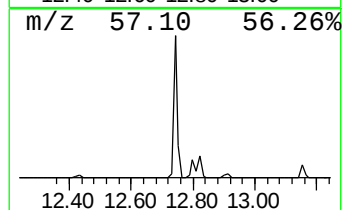
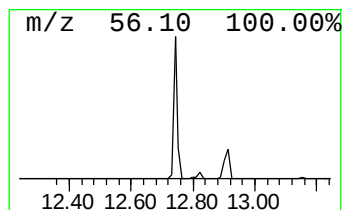
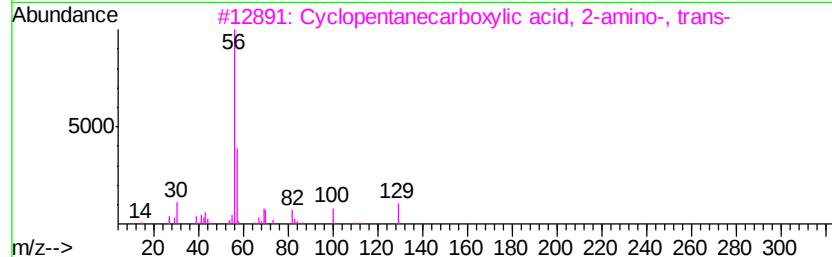
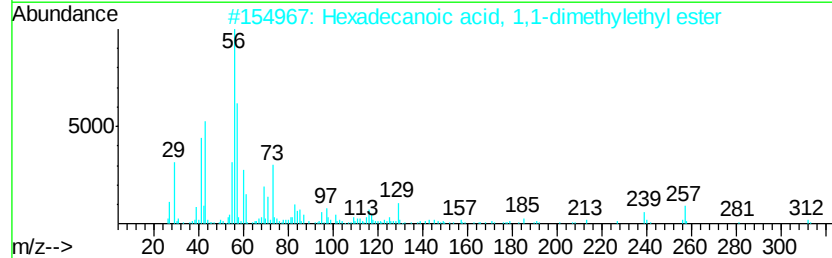
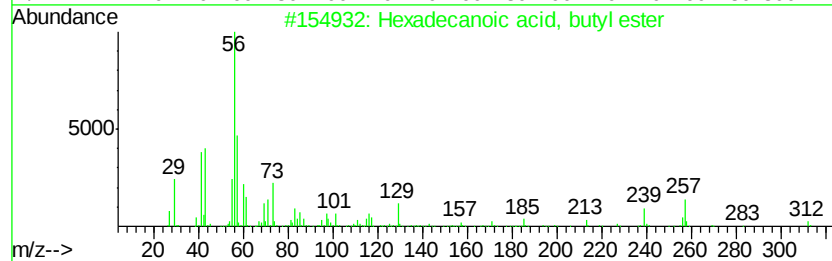
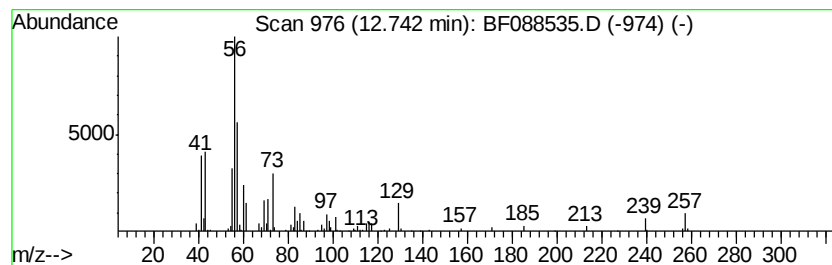
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.62 ng	258979	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



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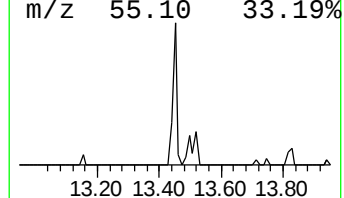
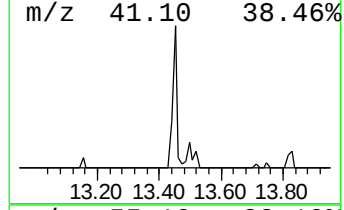
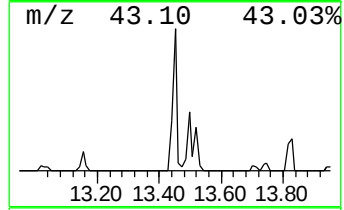
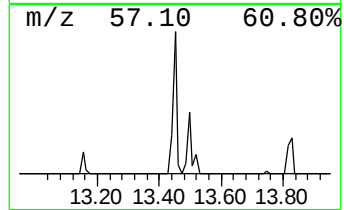
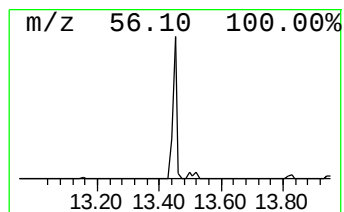
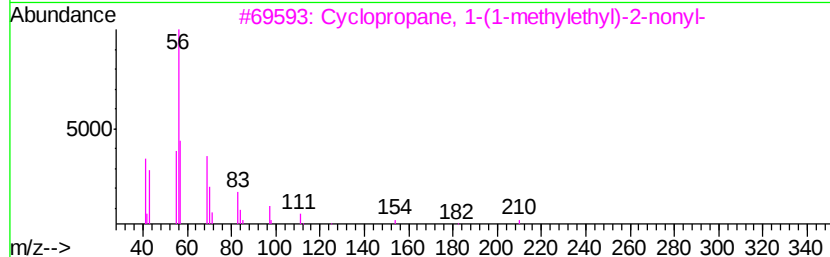
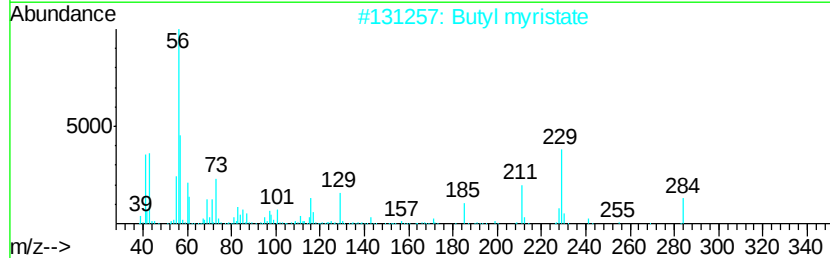
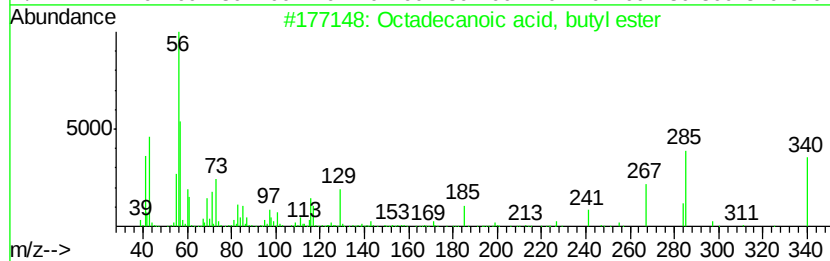
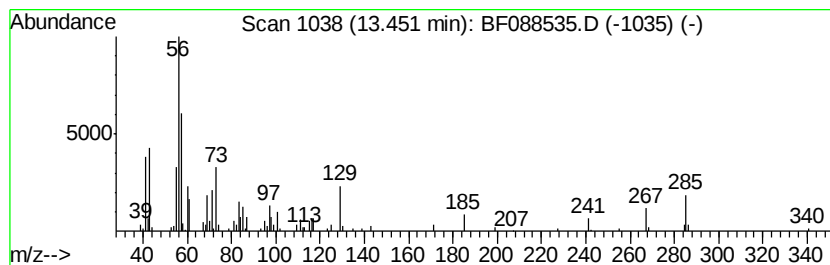
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Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.23 ng	159577	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		Butyl myristate	284	C18H36O2	000110-36-1	45
3		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	32



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.34	26.7	ng	1231190	1	6.81	922373	20.0
2-Pentanone, 4-hy...	5.00	32.8	ng	1511250	1	6.81	922373	20.0
unknown6.58	6.58	77.1	ng	3557750	1	6.81	922373	20.0
Hexadecanoic acid...	12.74	3.6	ng	258979	5	13.95	1429570	20.0
Octadecanoic acid...	13.45	2.2	ng	159577	5	13.95	1429570	20.0