

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
 Data File : BF088559.D
 Acq On : 1 Jul 2016 5:40
 Operator : UM/SJ
 Sample : H3747-04
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D9-B1(0-11)C

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-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	1.655	4	6	9	rVB	1992332	2020477	51.19%	7.696%
2	1.747	12	14	23	rVB	188774	418023	10.59%	1.592%
3	1.873	23	25	40	rVB	2303867	3946928	100.00%	15.035%
4	2.067	40	42	75	rVB	103199	490577	12.43%	1.869%
5	4.981	295	297	300	rBV	149540	207788	5.26%	0.792%
6	5.404	332	334	337	rBV	1282337	1833228	46.45%	6.983%
7	6.444	422	425	427	rBV	1966344	1878767	47.60%	7.157%
8	6.582	434	437	439	rBV	2094795	1879662	47.62%	7.160%
9	6.822	455	458	460	rBV	808891	855606	21.68%	3.259%
10	6.970	469	471	474	rVB	1457516	1486269	37.66%	5.662%
11	7.382	504	507	509	rBV	1270954	1363267	34.54%	5.193%
12	8.102	568	570	572	rBV	1390914	1146667	29.05%	4.368%
13	9.176	662	664	667	rBV	2188992	2024181	51.28%	7.711%
14	9.565	696	698	701	rVB	82142	100734	2.55%	0.384%
15	9.851	721	723	726	rBV	1266697	1173564	29.73%	4.470%
16	10.639	789	792	794	rBV	746800	885073	22.42%	3.371%
17	10.742	798	801	802	rBV	49979	57836	1.47%	0.220%
18	11.211	840	842	844	rBV	51840	47108	1.19%	0.179%
19	11.325	850	852	855	rBV	772211	1000472	25.35%	3.811%
20	12.754	974	977	980	rBV2	44803	82220	2.08%	0.313%
21	12.914	989	991	993	rBV	1627408	1409073	35.70%	5.367%
22	13.828	1068	1071	1075	rBV	155829	241172	6.11%	0.919%
23	13.954	1080	1082	1085	rVB	839148	849945	21.53%	3.238%
24	14.148	1097	1099	1100	rBV	32247	51359	1.30%	0.196%
25	15.360	1202	1205	1208	rVB	624065	802197	20.32%	3.056%

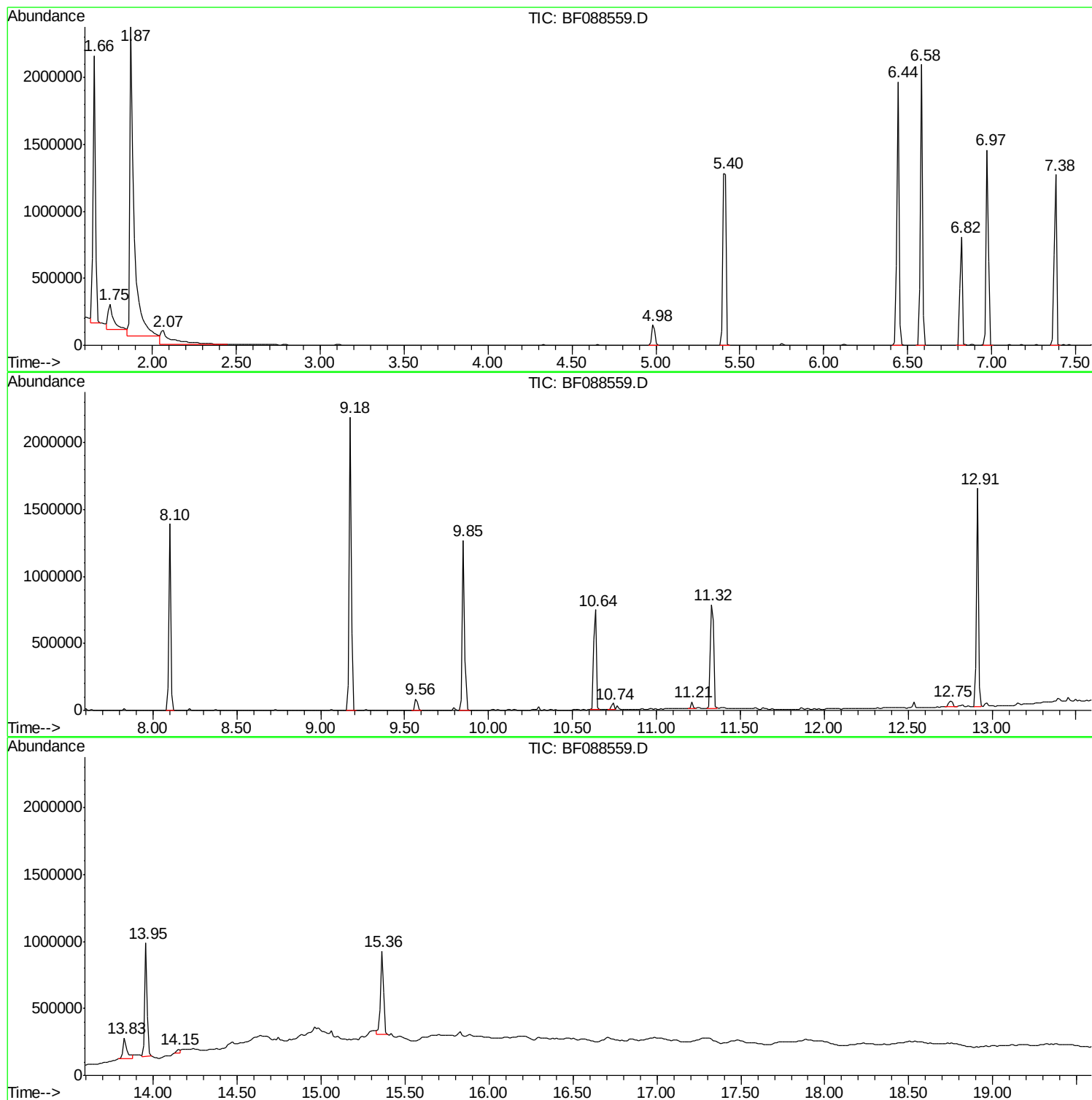
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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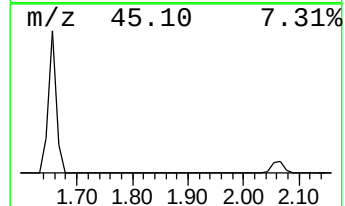
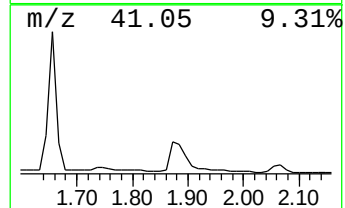
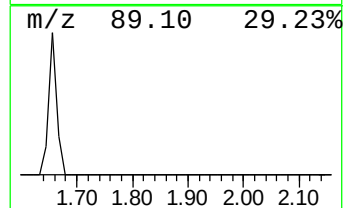
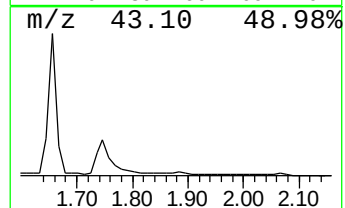
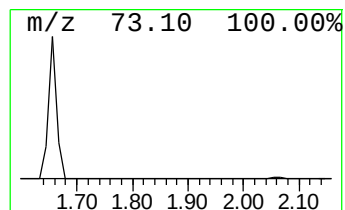
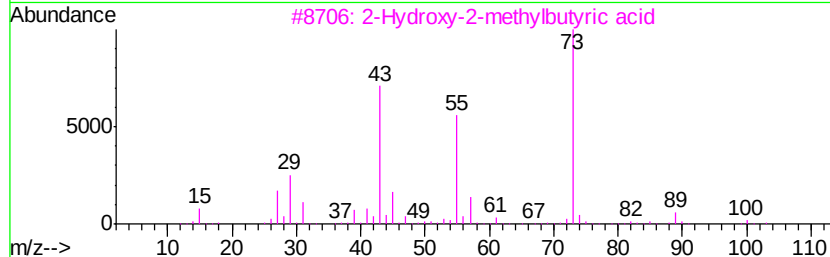
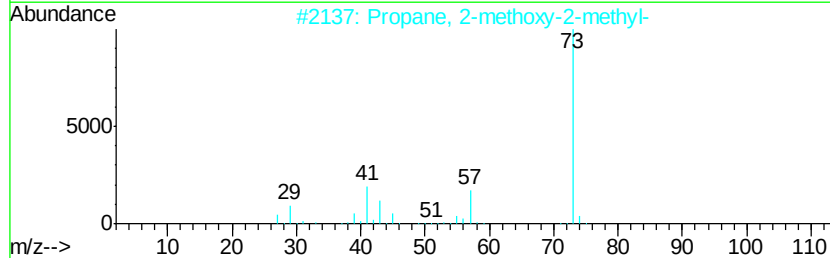
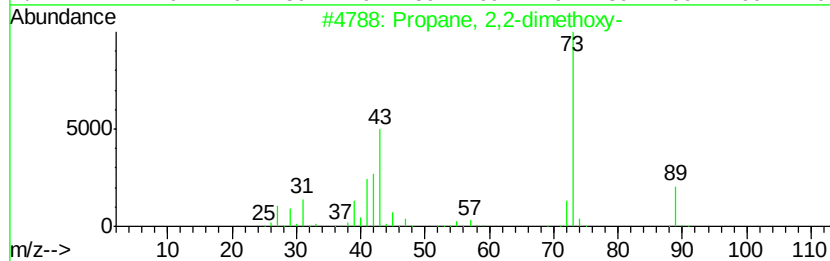
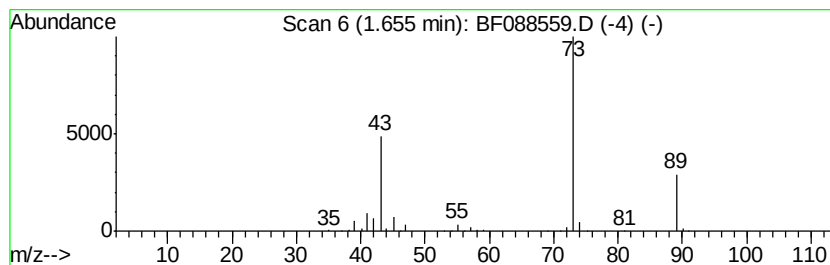
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	47.23 ng	2020480	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



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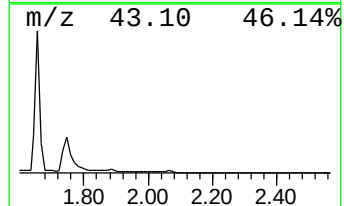
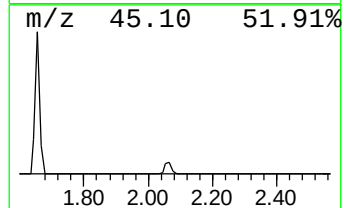
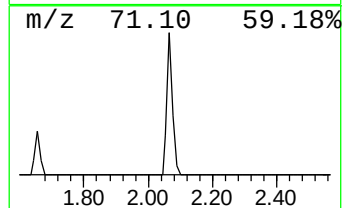
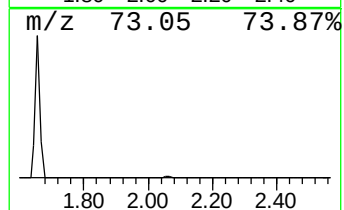
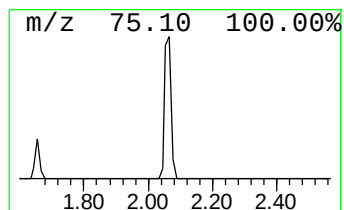
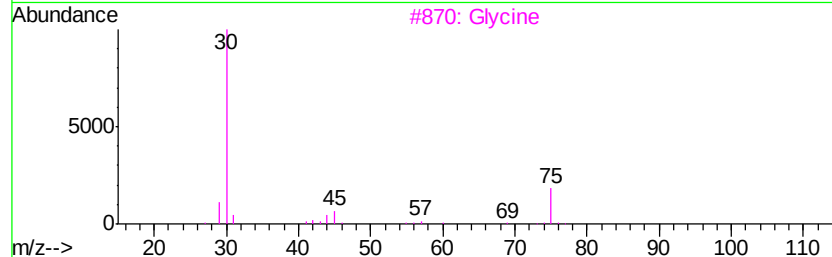
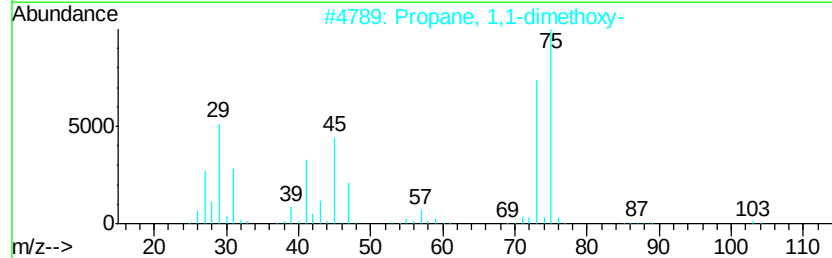
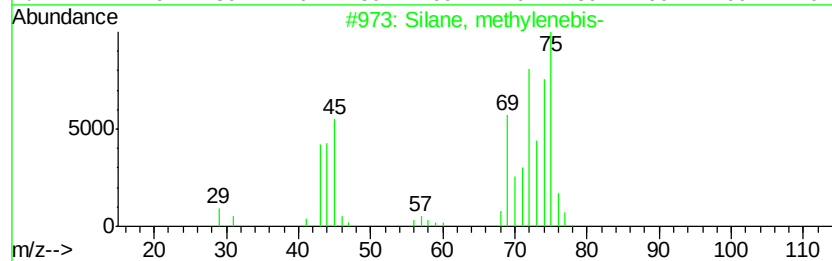
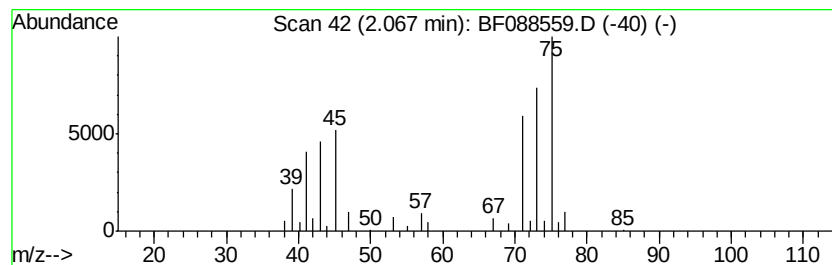
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown2.07 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	11.47 ng	490577	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silane, methylenebis-	76	CH8Si2	001759-88-2	45
2		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	42
3		Glycine	75	C2H5NO2	000056-40-6	9
4		trans-2-Methyl-4-hexen-3-ol	114	C7H14O	096346-76-8	9
5		Oxirane, butyl-	100	C6H12O	001436-34-6	9



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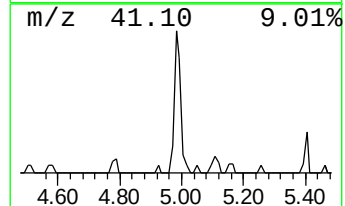
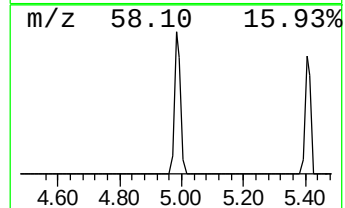
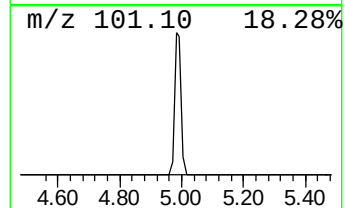
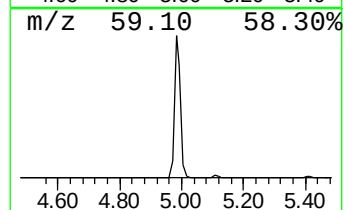
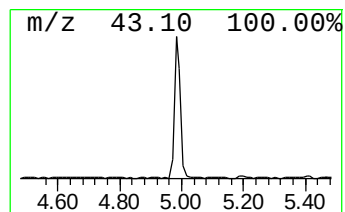
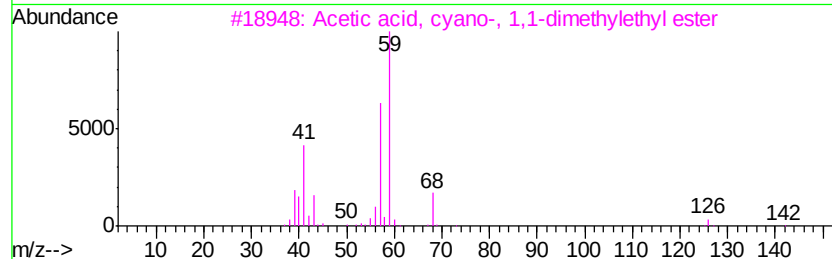
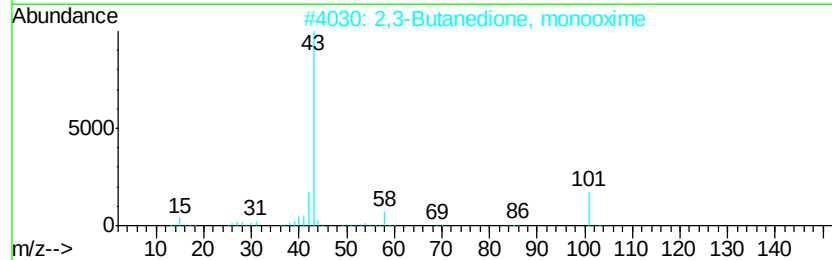
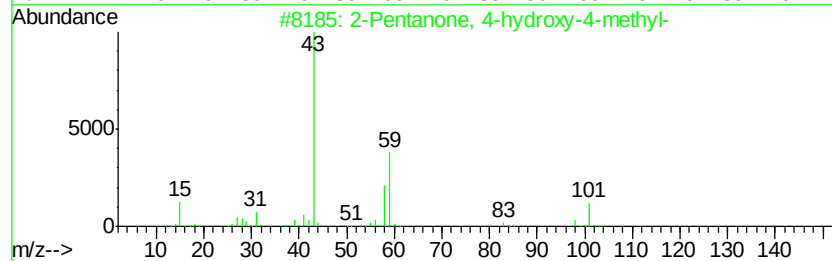
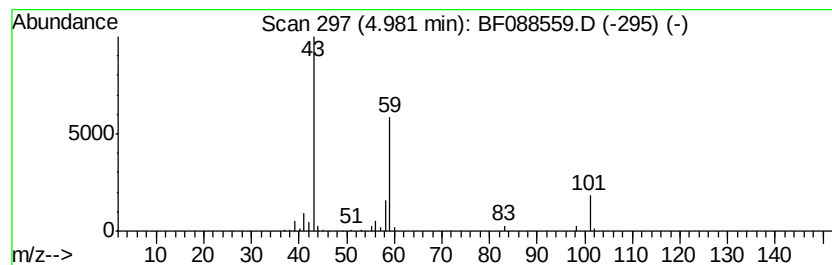
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	4.86 ng	207788	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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-dimethyl...	141	C7H11NO2	001116-98-9	25		
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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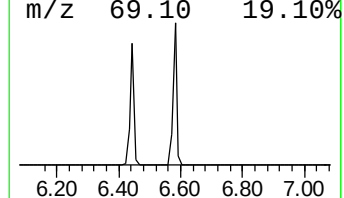
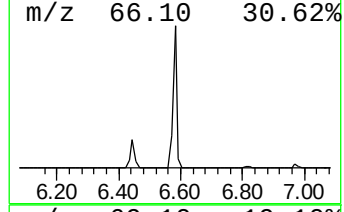
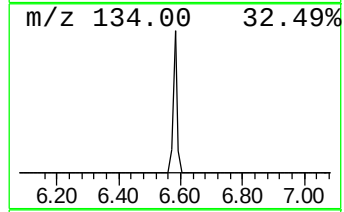
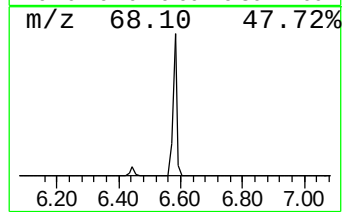
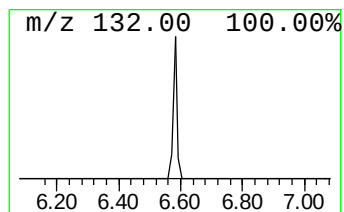
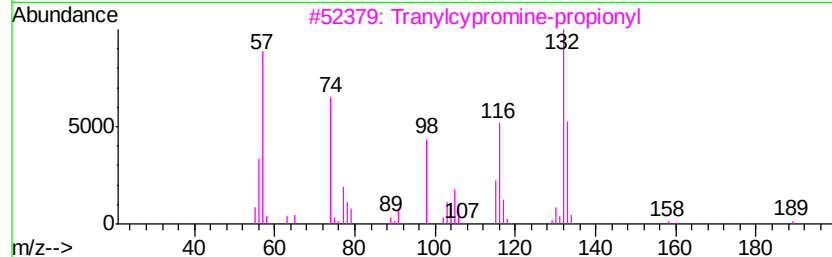
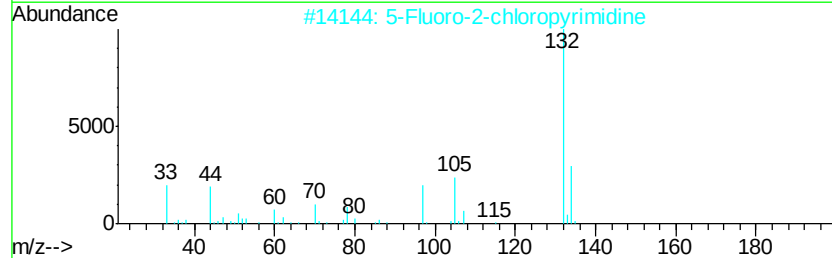
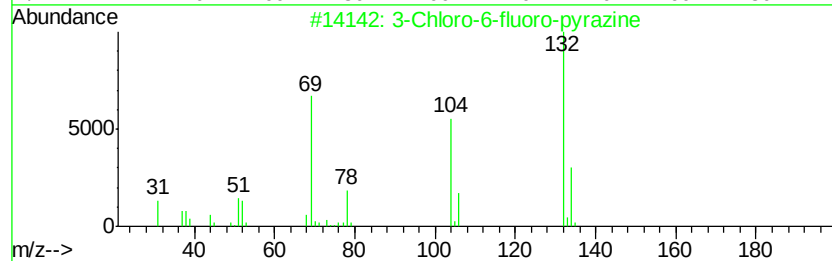
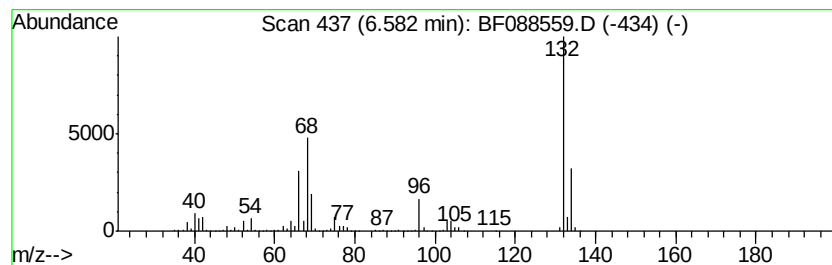
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Peak Number 6 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	43.94 ng	1879660	1,4-Dichlorobenzene-d4	6.82

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	27
3		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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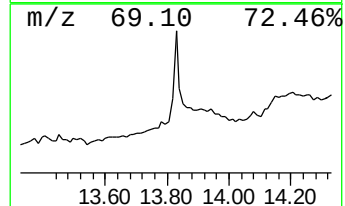
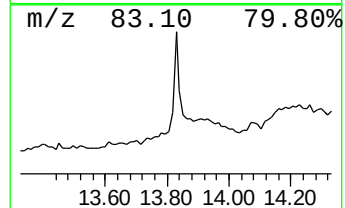
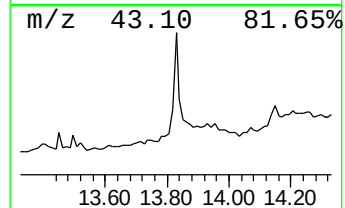
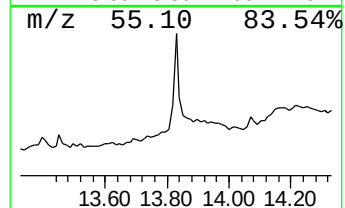
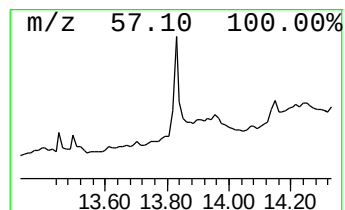
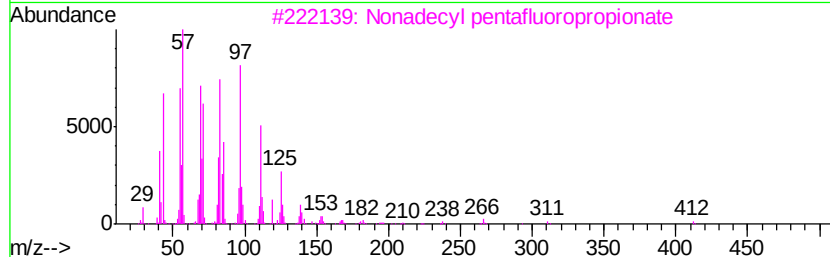
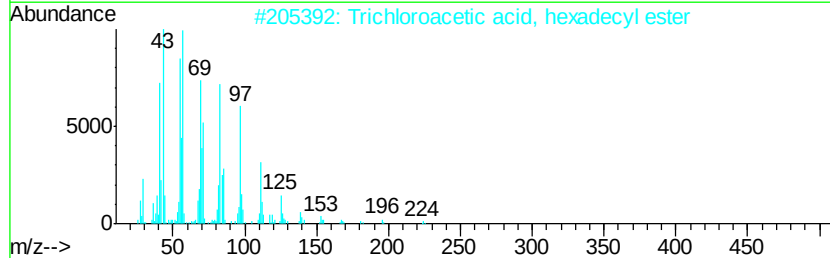
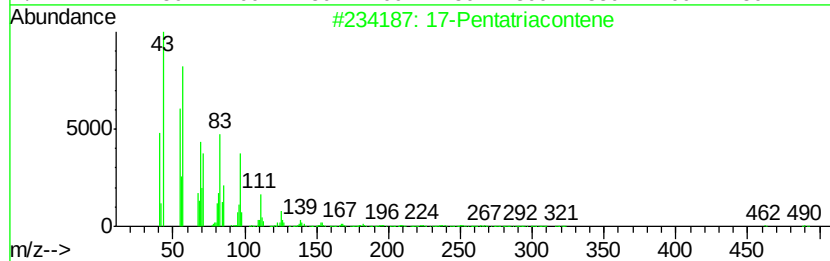
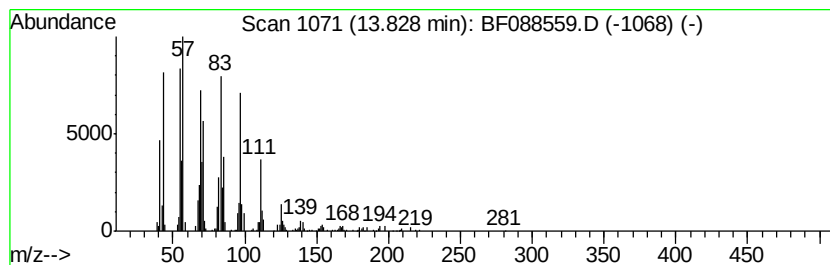
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Peak Number 8 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.83	5.68 ng	241172	Chrysene-d12	13.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
4	Behenic alcohol	326	C22H46O	000661-19-8	76
5	1-Heneicosanol	312	C21H44O	015594-90-8	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.66	47.2	ng	2020480	1	6.82	855606	20.0
unknown2.07	2.07	11.5	ng	490577	1	6.82	855606	20.0
2-Pentanone, 4-hy...	4.98	4.9	ng	207788	1	6.82	855606	20.0
unknown6.58	6.58	43.9	ng	1879660	1	6.82	855606	20.0
17-Pentatriacontene	13.83	5.7	ng	241172	5	13.95	849945	20.0