

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088606.D
Acq On : 2 Jul 2016 6:57
Operator : UM/SJ
Sample : H3831-12
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-21-COMP

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	1.678	4	8	10	rVB	5001332	7866314	100.00%	19.853%
2	1.735	11	13	23	rVB	657239	1048573	13.33%	2.646%
3	1.861	23	24	40	rVB	2447023	5284044	67.17%	13.336%
4	2.067	40	42	83	rVB	136080	755109	9.60%	1.906%
5	4.981	295	297	301	rBV	194983	285204	3.63%	0.720%
6	5.404	331	334	337	rBV	2342790	2606259	33.13%	6.578%
7	6.444	421	425	427	rBV	2628767	3164921	40.23%	7.988%
8	6.570	434	436	439	rBV	2217652	2836533	36.06%	7.159%
9	6.810	454	457	459	rBV	838664	806213	10.25%	2.035%
10	6.959	468	470	473	rVB	1665762	2283048	29.02%	5.762%
11	7.370	503	506	508	rBV	1825940	1775463	22.57%	4.481%
12	8.090	566	569	571	rVB	1227004	1038486	13.20%	2.621%
13	9.165	661	663	666	rVB	2224038	2995347	38.08%	7.560%
14	9.565	696	698	700	rBV	136365	149453	1.90%	0.377%
15	9.839	720	722	725	rVB	1065580	987694	12.56%	2.493%
16	10.628	788	791	793	rBV	1410085	1445636	18.38%	3.648%
17	11.313	849	851	854	rVB	667422	813063	10.34%	2.052%
18	12.902	987	990	993	rBV	2304578	2095938	26.64%	5.290%
19	13.828	1068	1071	1079	rBV	49267	112241	1.43%	0.283%
20	13.942	1079	1081	1083	rBV	833147	713500	9.07%	1.801%
21	15.337	1201	1203	1206	rBV	383295	560150	7.12%	1.414%

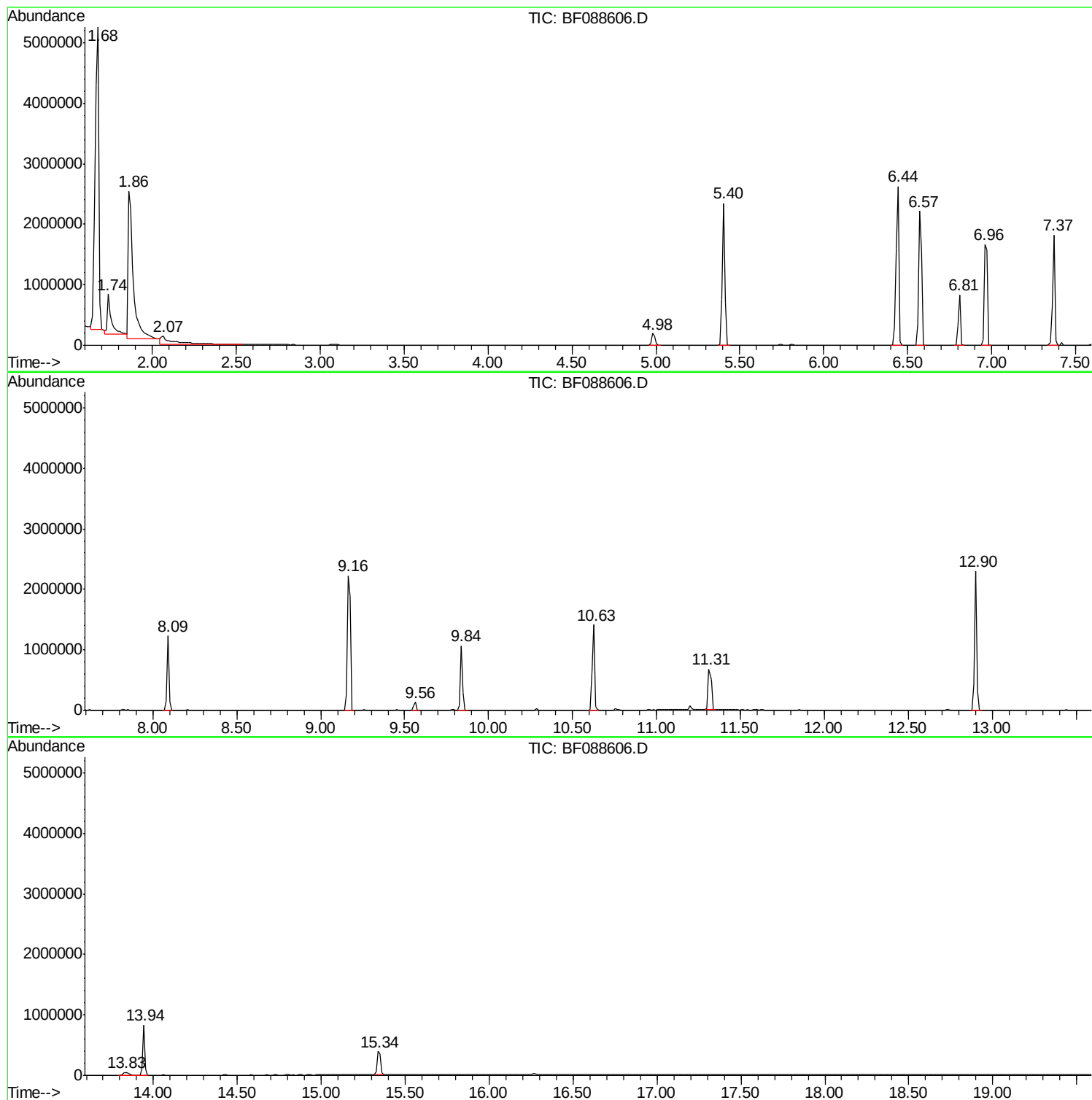
Sum of corrected areas: 39623189

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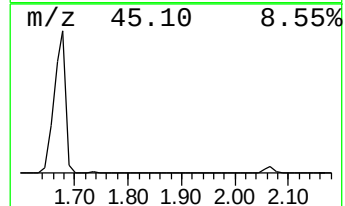
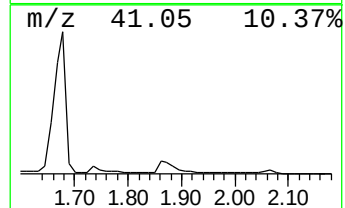
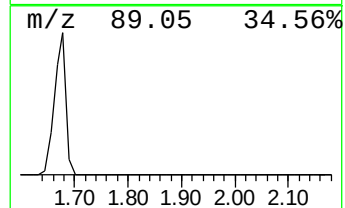
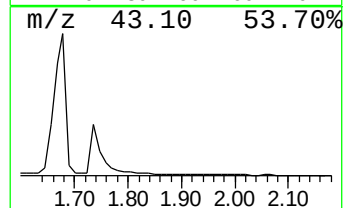
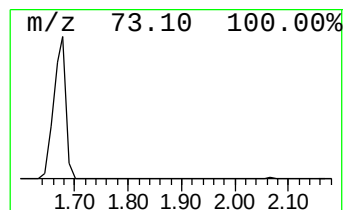
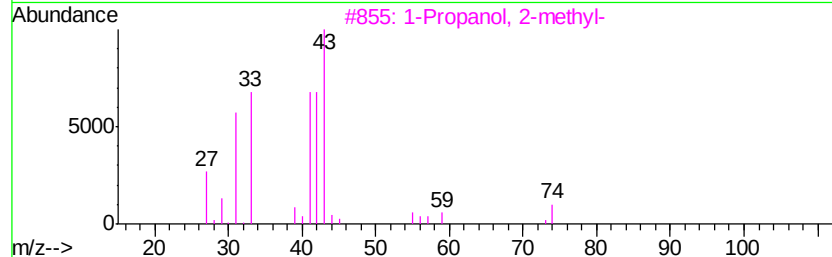
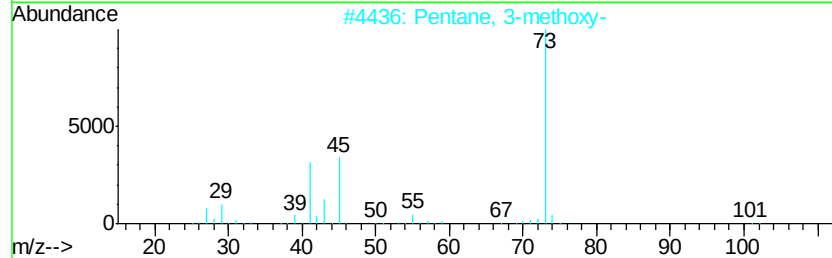
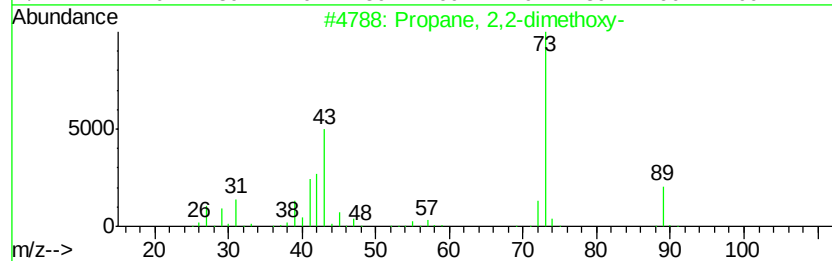
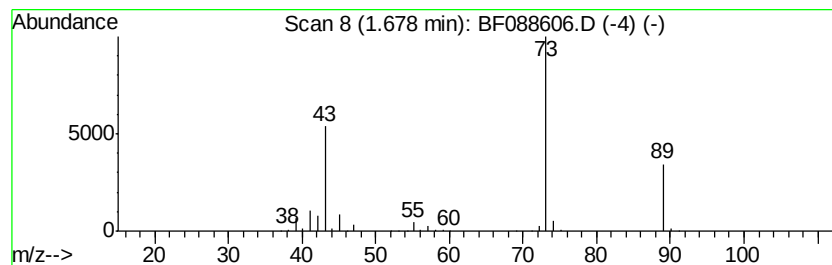
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Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	195.14 ng	7866310	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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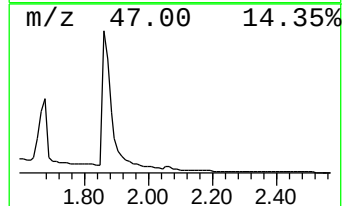
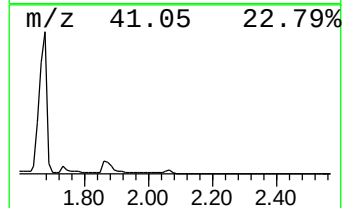
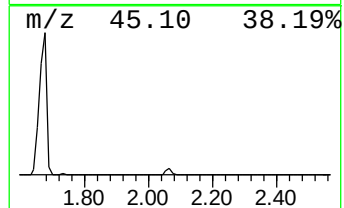
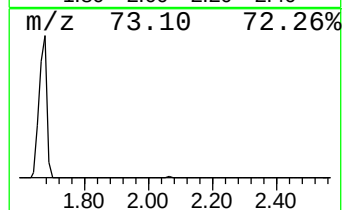
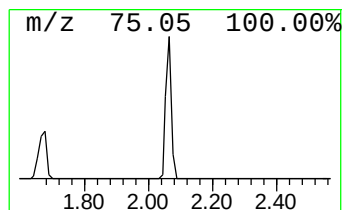
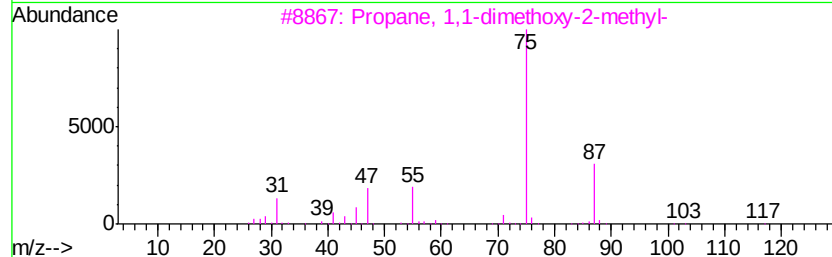
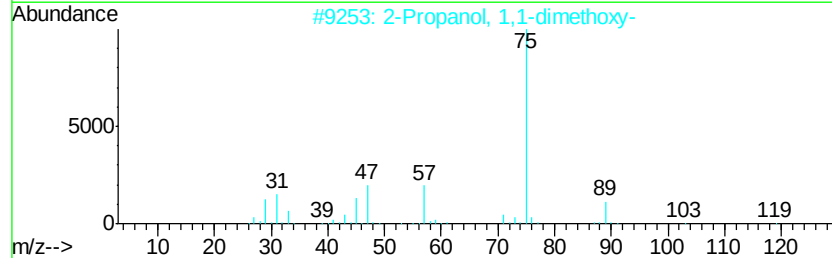
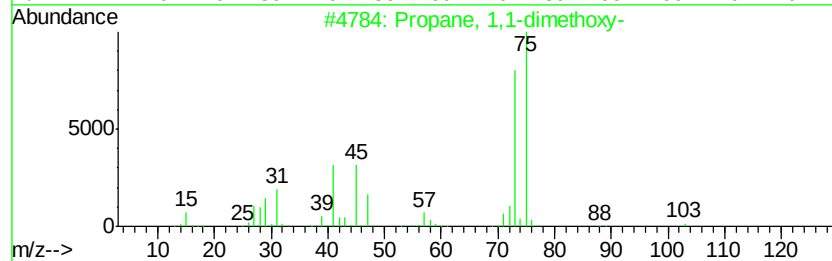
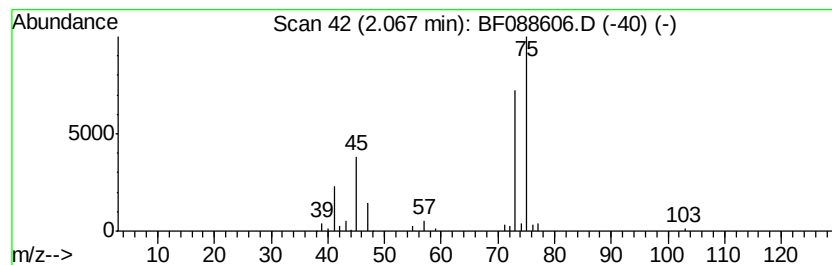
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Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	18.73 ng	755109	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	33
3			Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	28
4			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
5			Chloromethyl cyanide	75	C2H2ClN	000107-14-2	9



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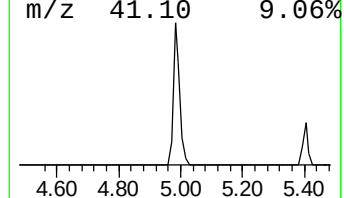
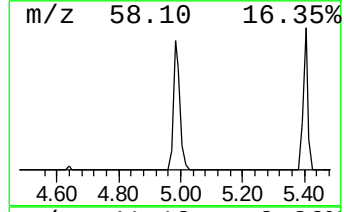
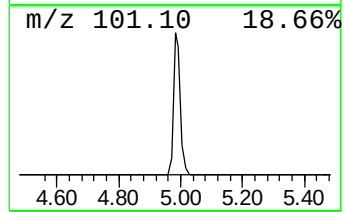
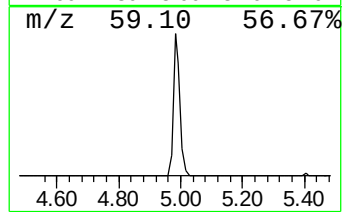
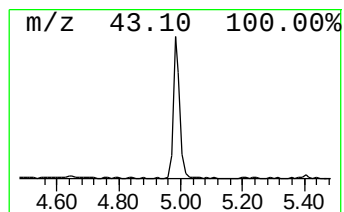
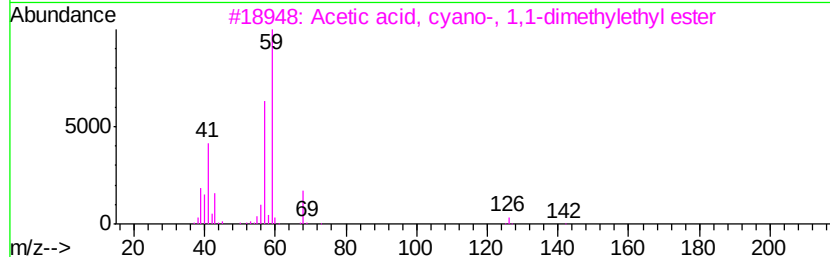
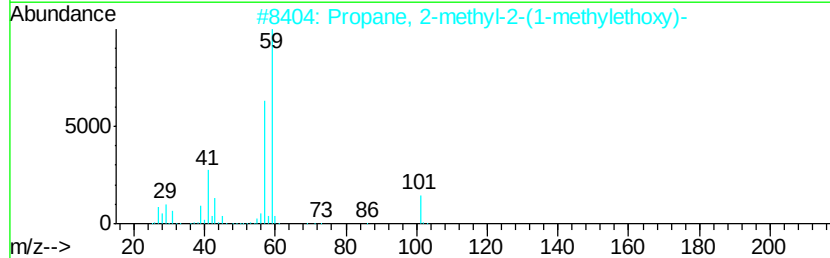
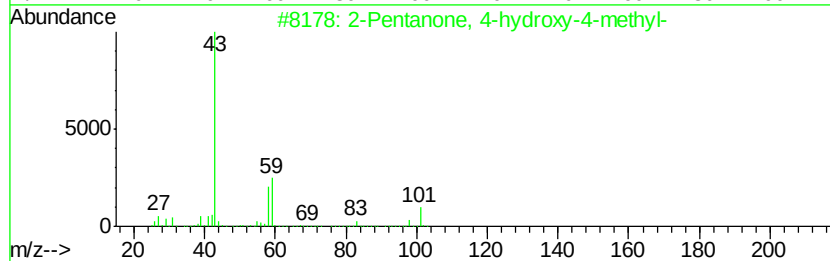
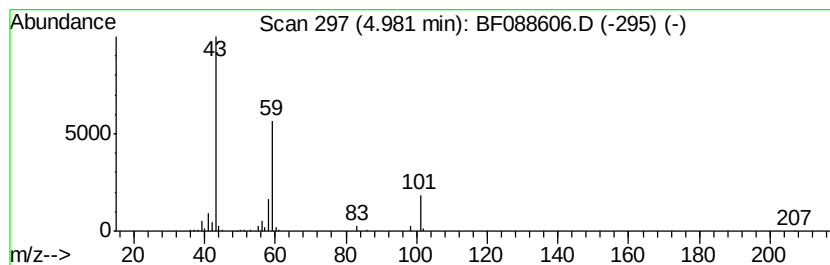
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	7.08 ng	285204	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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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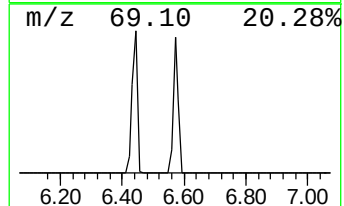
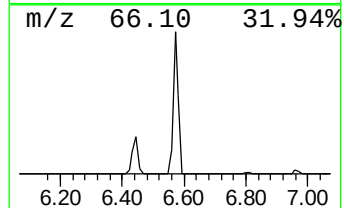
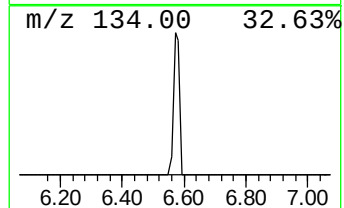
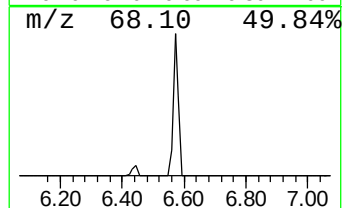
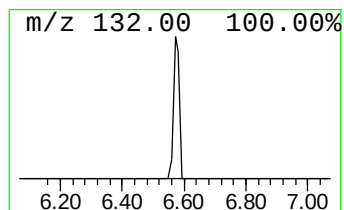
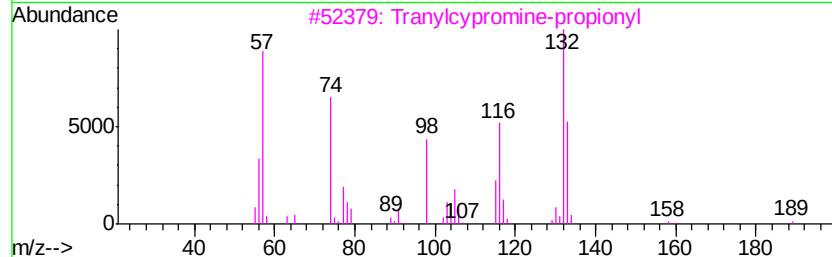
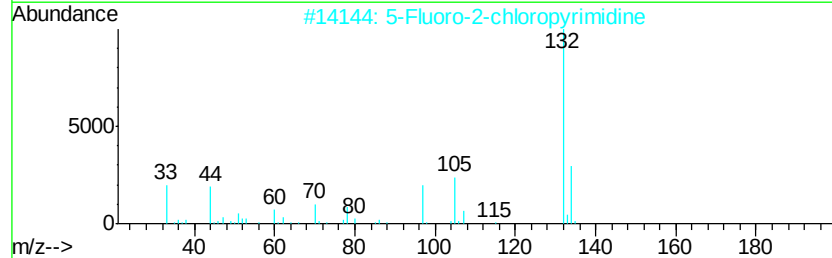
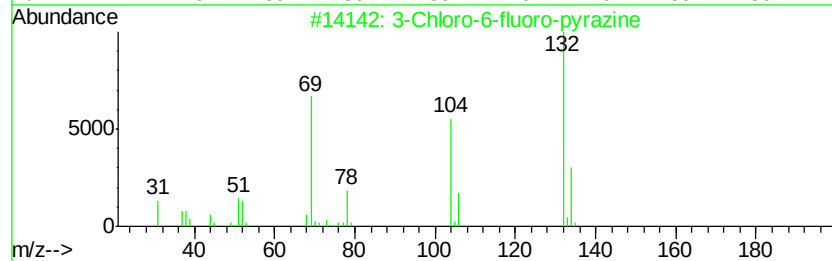
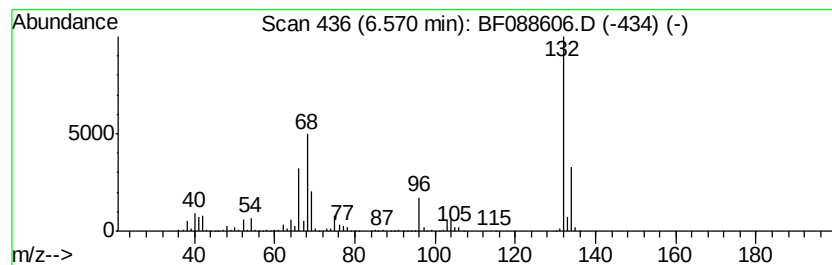
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Peak Number 6 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	70.37 ng	2836530	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	12
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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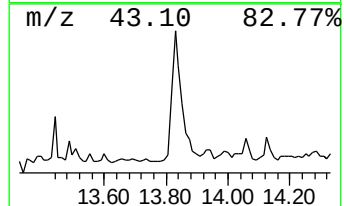
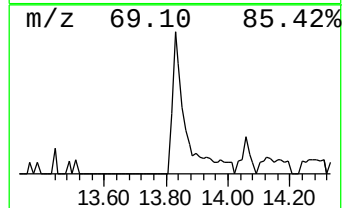
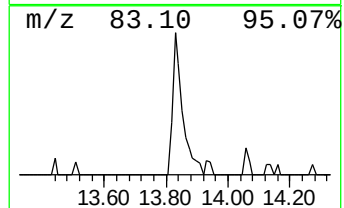
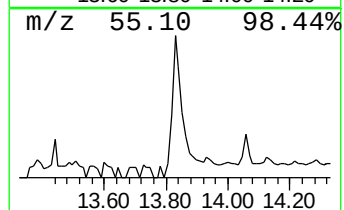
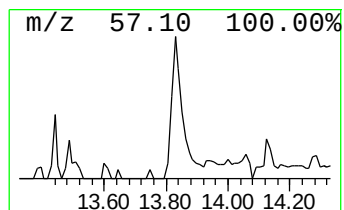
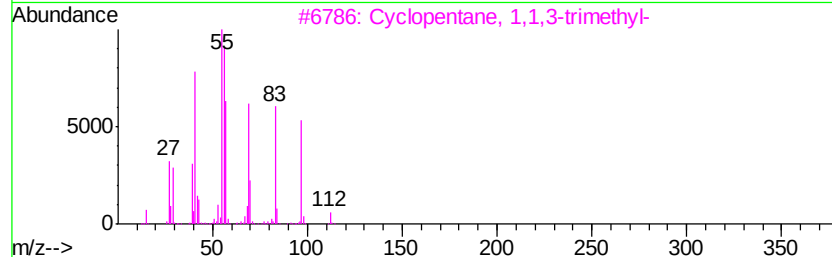
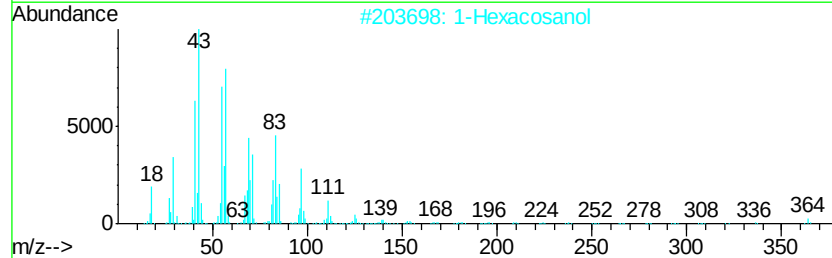
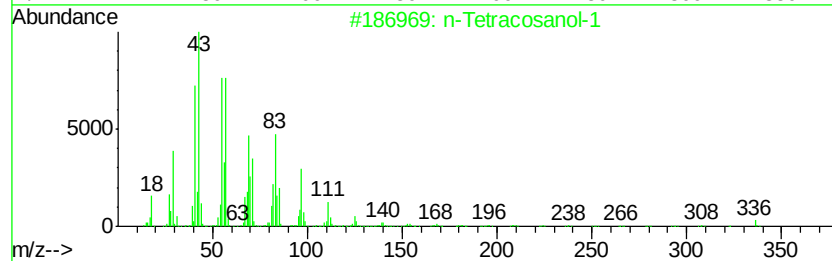
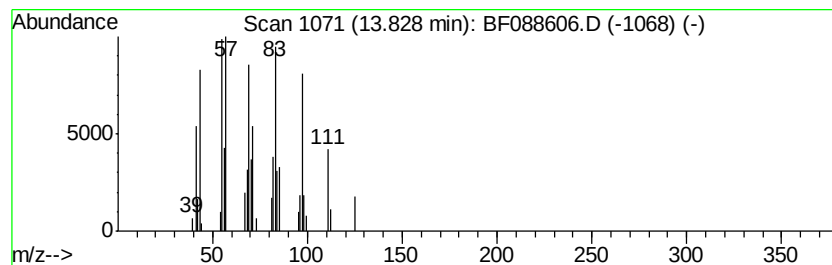
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Peak Number 8 n-Tetracosanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.83	3.15 ng	112241	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	62
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	49
4	Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	38
5	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.68	195.1	ng	7866310	1	6.81	806213	20.0
Propane, 1,1-dime...	2.07	18.7	ng	755109	1	6.81	806213	20.0
2-Pentanone, 4-hy...	4.98	7.1	ng	285204	1	6.81	806213	20.0
unknown6.57	6.57	70.4	ng	2836530	1	6.81	806213	20.0
n-Tetracosanol-1	13.83	3.1	ng	112241	5	13.94	713500	20.0