

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092815\
 Data File : BF081863.D
 Acq On : 29 Sep 2015 3:30
 Operator : UM/IZ
 Sample : G3717-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-3-9-16-15

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-BF092815.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	5.108	257	260	266	rBV	214008	335356	9.14%	1.348%
2	5.520	293	296	315	rBV	587938	1049308	28.61%	4.219%
3	6.549	384	386	396	rBV	412234	694575	18.94%	2.792%
4	6.697	396	399	401	rBV	1826130	2170943	59.19%	8.728%
5	6.937	418	420	428	rBV	373934	645168	17.59%	2.594%
6	7.086	431	433	448	rVB	2224340	2389554	65.15%	9.607%
7	7.497	466	469	483	rBV	1571465	1979262	53.96%	7.957%
8	8.217	530	532	546	rBV	673430	894000	24.37%	3.594%
9	9.303	624	627	629	rBV	2427135	3611179	98.46%	14.518%
10	9.692	659	661	667	rBV	113211	136167	3.71%	0.547%
11	9.978	683	686	698	rBV	897477	991840	27.04%	3.988%
12	10.400	719	723	725	rBV	31149	40708	1.11%	0.164%
13	10.766	752	755	763	rBV	2114118	2425777	66.14%	9.753%
14	10.869	763	764	769	rVB2	33173	67498	1.84%	0.271%
15	10.972	772	773	775	rVV2	31386	39460	1.08%	0.159%
16	11.155	788	789	792	rBV4	28401	39221	1.07%	0.158%
17	11.326	801	804	807	rBV2	21491	44481	1.21%	0.179%
18	11.463	814	816	826	rVB	956156	1050485	28.64%	4.223%
19	11.806	844	846	853	rVB	87865	119605	3.26%	0.481%
20	11.989	859	862	864	rBV2	40808	58864	1.60%	0.237%
21	12.869	935	939	944	rBV2	95488	112047	3.05%	0.450%
22	13.052	952	955	958	rBV	3162012	3667741	100.00%	14.746%
23	13.578	998	1001	1003	rBV	68489	80334	2.19%	0.323%
24	13.646	1005	1007	1015	rVV	316363	396204	10.80%	1.593%
25	13.967	1032	1035	1039	rBV	50089	110473	3.01%	0.444%
26	14.104	1045	1047	1050	rBV	881523	960173	26.18%	3.860%
27	15.578	1173	1176	1186	rVB	545049	762769	20.80%	3.067%

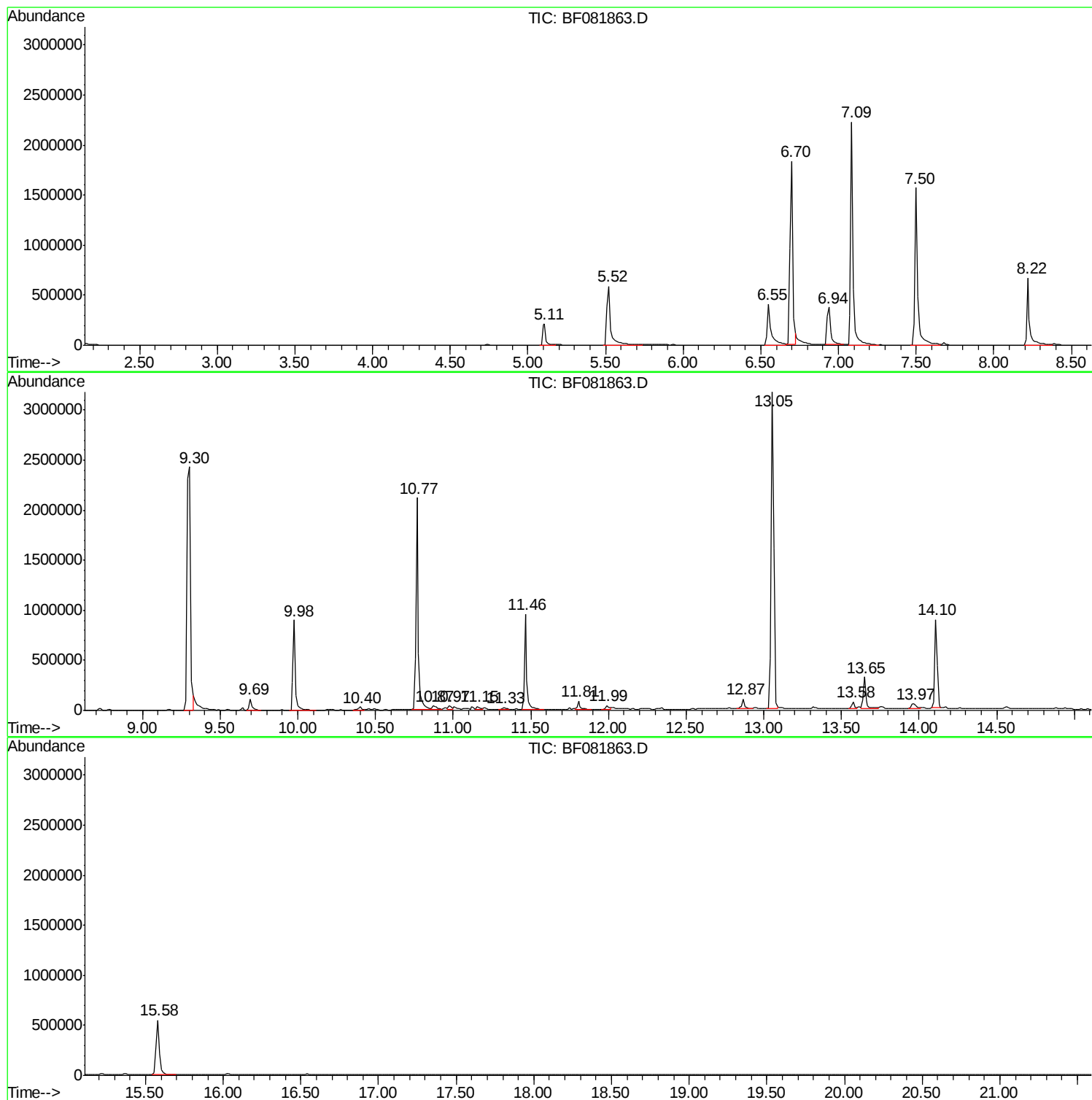
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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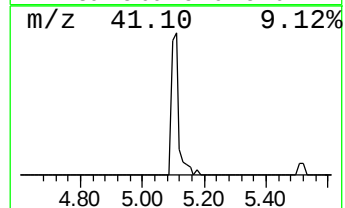
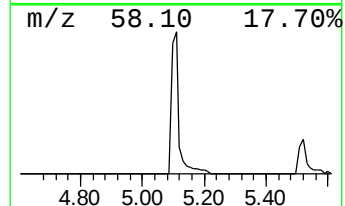
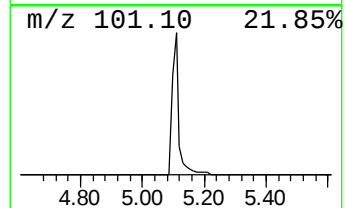
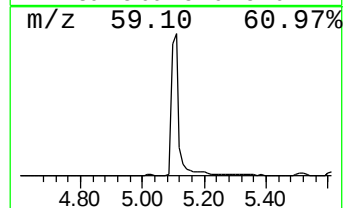
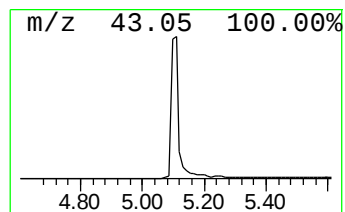
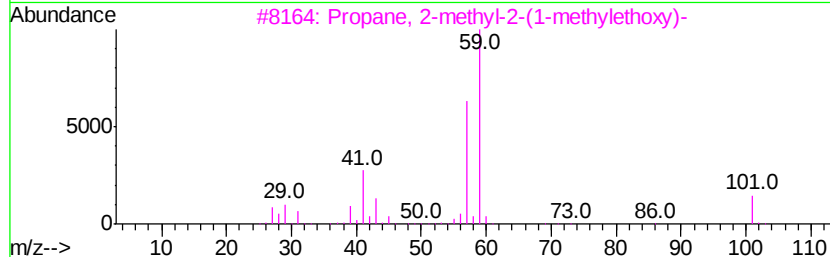
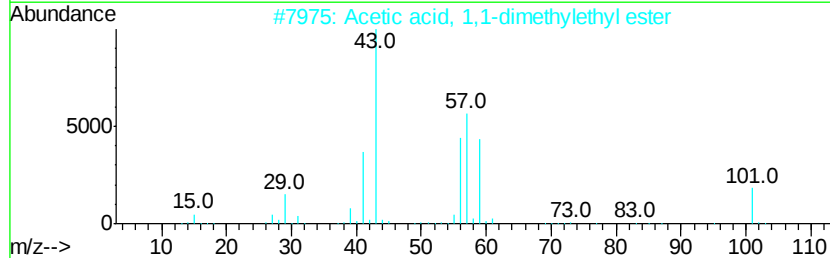
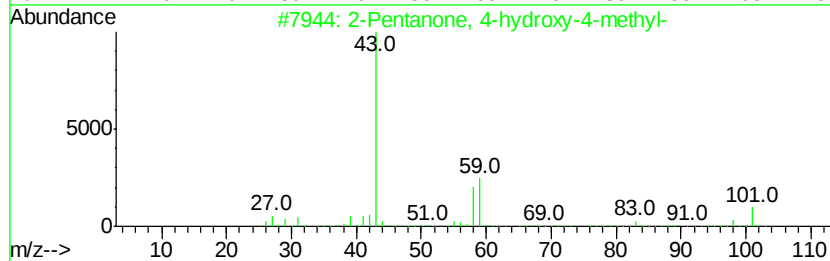
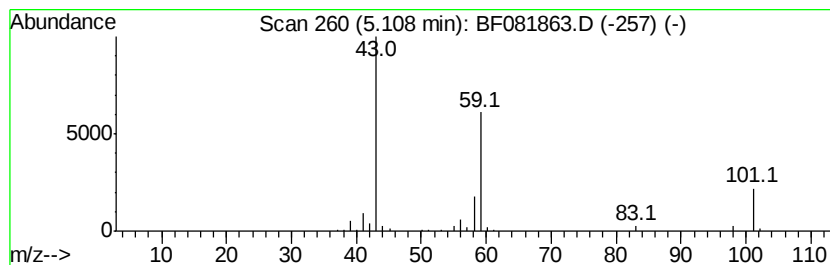
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	10.40 ng	335356	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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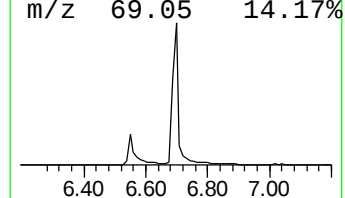
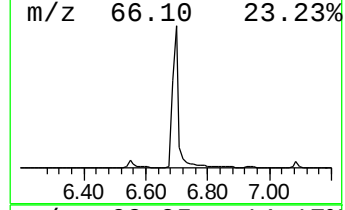
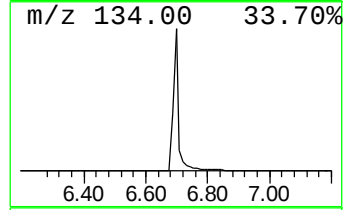
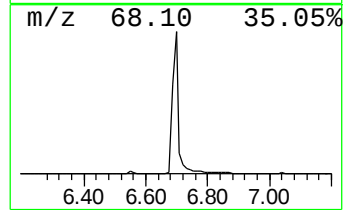
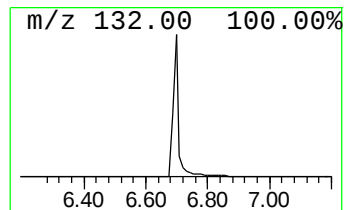
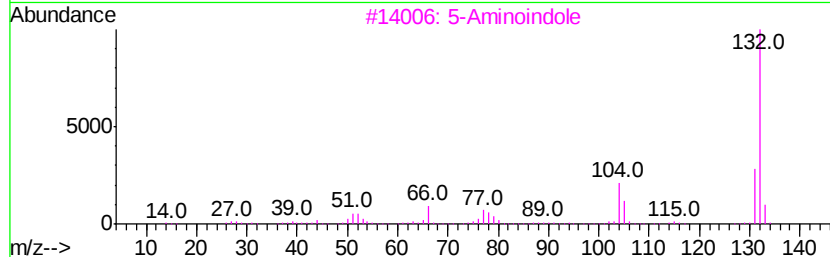
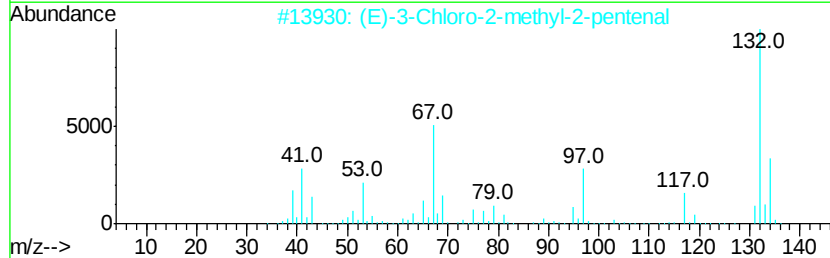
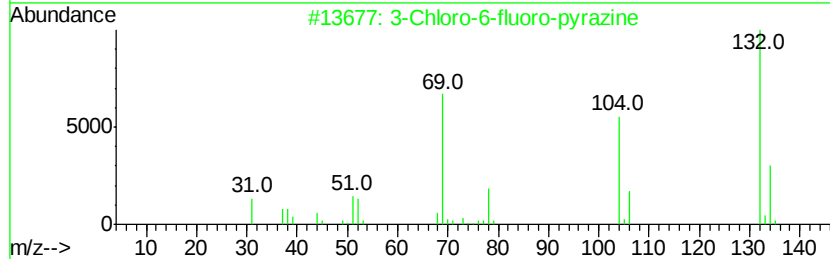
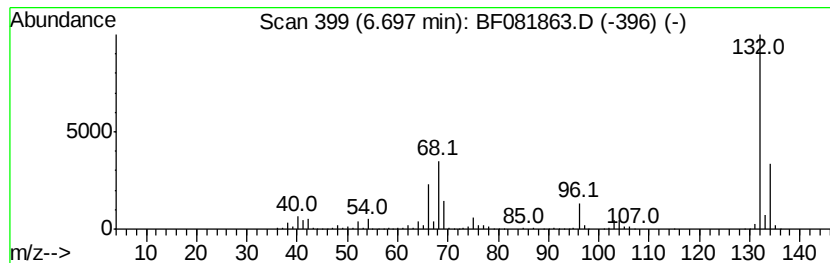
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Peak Number 2 unknown6.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	67.30 ng	2170940	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



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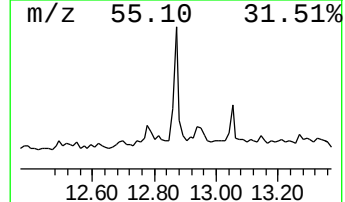
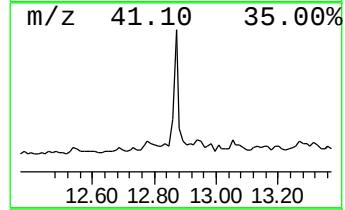
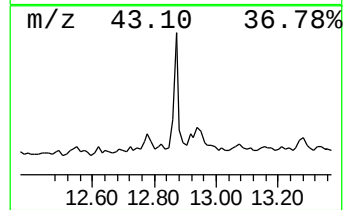
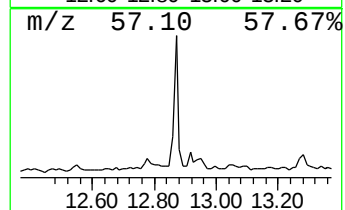
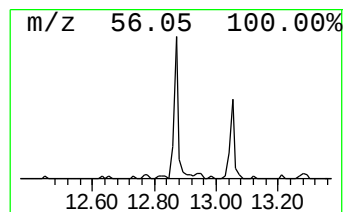
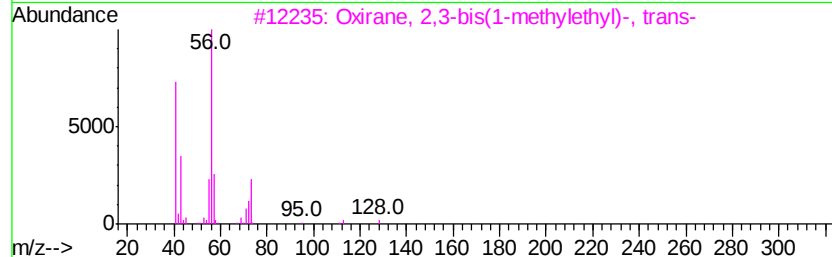
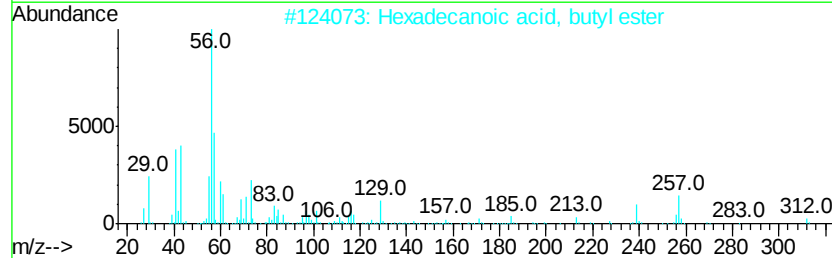
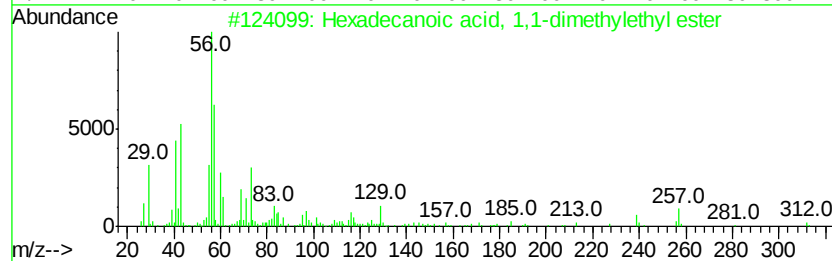
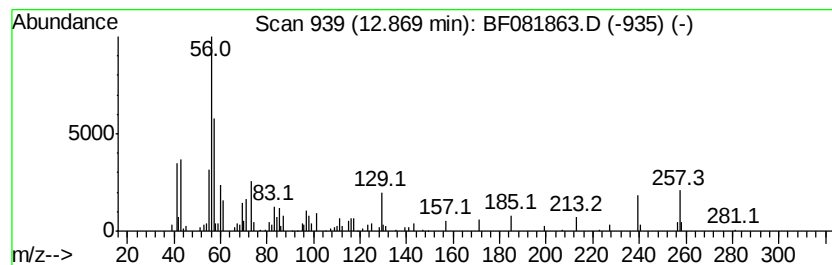
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.33 ng	112047	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	43
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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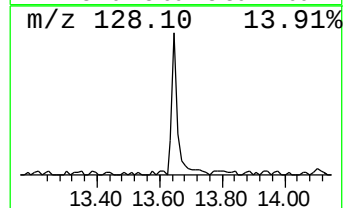
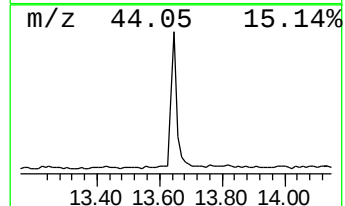
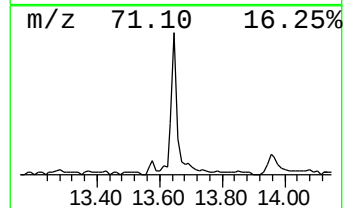
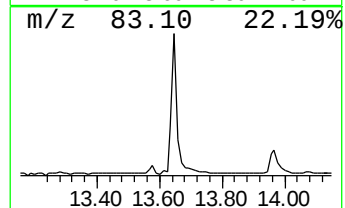
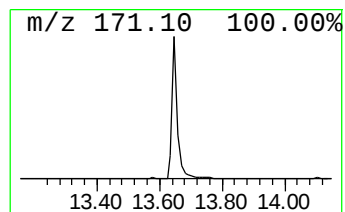
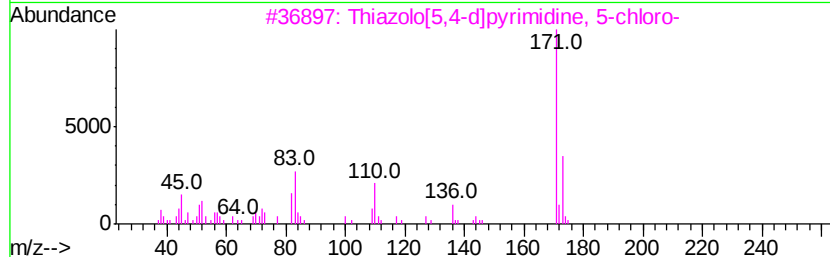
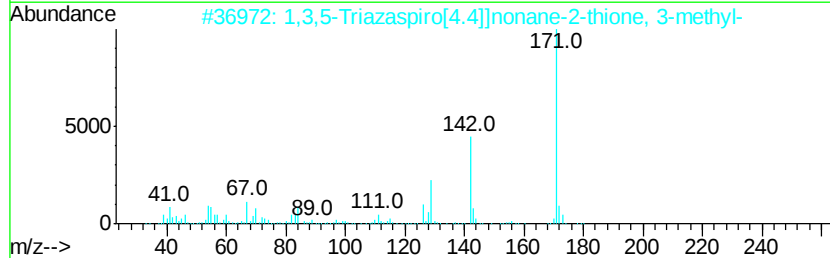
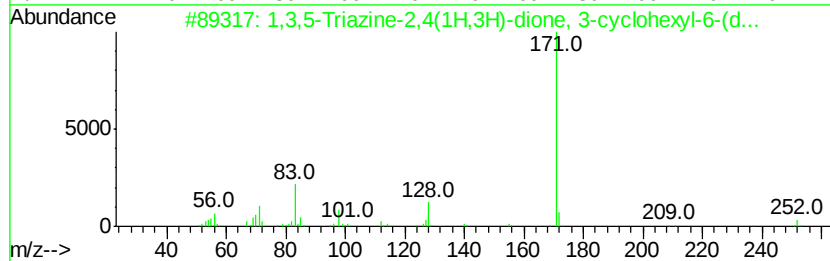
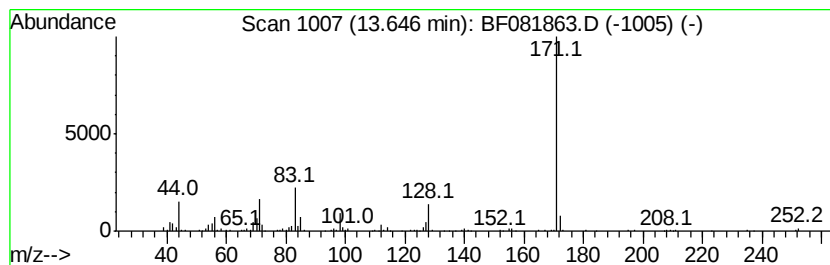
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Peak Number 6 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	8.25 ng	396204	Chrysene-d12	14.10
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252 C12H20N4O2	051235-04-2	91
2	1,3,5-Triazaspiro[4.4]nonane-2-...	171 C7H13N3S	1000277-58-6	40
3	Thiazolo[5,4-d]pyrimidine, 5-chl...	171 C5H2ClN3S	013316-08-0	38
4	Benzeneethanamine, 2-fluoro-4-hv...	171 C8H10FN02	1000116-43-3	33
5	4-Pyridinol, 2-phenyl-	171 C11H9NO	1000253-54-5	28



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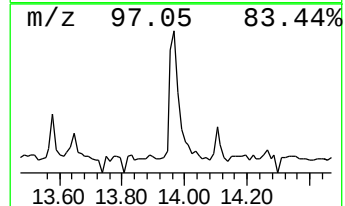
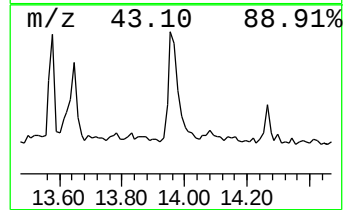
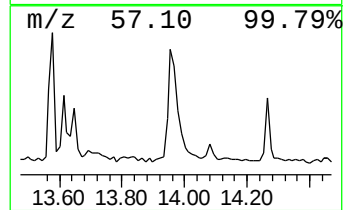
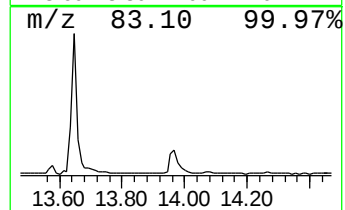
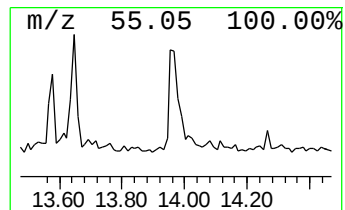
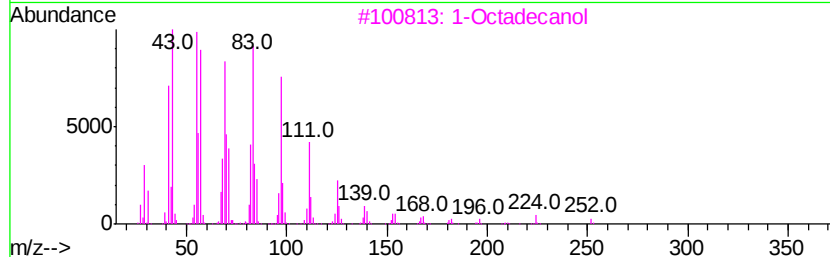
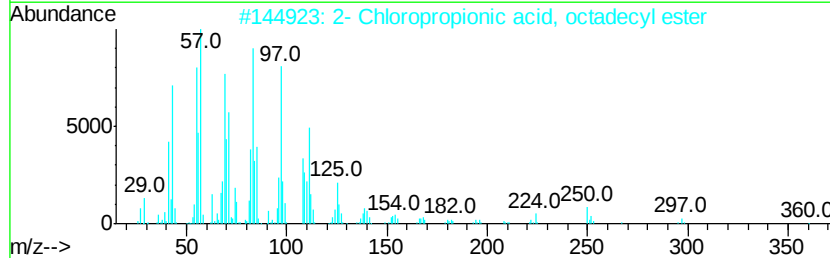
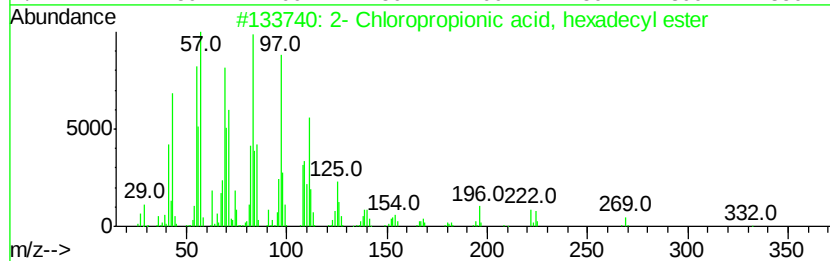
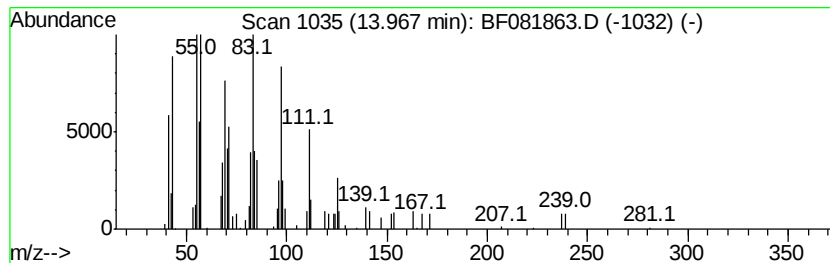
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Peak Number 7 2- Chloropropionic acid, he... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.30 ng	110473	Chrysene-d12	14.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-		Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
2	2-		Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
3	1-		Octadecanol	270	C18H38O	000112-92-5	91
4	2-		Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	10.4	ng	335356	1	6.94	645168	20.0
unknown6.70	6.70	67.3	ng	2170940	1	6.94	645168	20.0
Hexadecanoic acid...	12.87	2.3	ng	112047	5	14.10	960173	20.0
1,3,5-Triazine-2,...	13.65	8.3	ng	396204	5	14.10	960173	20.0
2- Chloropropioni...	13.97	2.3	ng	110473	5	14.10	960173	20.0