

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
 Data File : BF083845.D
 Acq On : 16 Dec 2015 13:50
 Operator : UM/SJ
 Sample : G4680-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 K202-(18-19)

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-BF121315.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	5.082	259	262	267	rBV	312532	486435	14.65%	1.895%
2	5.504	296	299	302	rBV	2076274	2240072	67.48%	8.725%
3	6.533	385	389	391	rBV	1976565	2676309	80.62%	10.424%
4	6.659	398	400	403	rBV	2143351	2422067	72.96%	9.434%
5	6.887	418	420	423	rBV	574393	514847	15.51%	2.005%
6	7.047	431	434	437	rBV	2153192	1970495	59.36%	7.675%
7	7.459	466	470	472	rBV	1159842	1708951	51.48%	6.656%
8	7.562	476	479	487	rVB	33946	55259	1.66%	0.215%
9	8.179	530	533	535	rBV	474944	656999	19.79%	2.559%
10	9.253	624	627	629	rBV	3284954	3319753	100.00%	12.930%
11	9.642	659	661	663	rBV	844251	691473	20.83%	2.693%
12	9.871	679	681	683	rVB	30325	36880	1.11%	0.144%
13	9.928	683	686	688	rBV	891665	806903	24.31%	3.143%
14	10.362	723	724	726	rVB	65149	56587	1.70%	0.220%
15	10.591	740	744	747	rBV	19078	37782	1.14%	0.147%
16	10.716	752	755	757	rBV	1938540	2019841	60.84%	7.867%
17	10.842	764	766	770	rVB	50650	85450	2.57%	0.333%
18	11.288	800	805	806	rBV	47708	57072	1.72%	0.222%
19	11.402	813	815	818	rVB	595121	772437	23.27%	3.009%
20	11.642	833	836	838	rBV	52491	79433	2.39%	0.309%
21	11.711	840	842	844	rVB	44765	37639	1.13%	0.147%
22	12.454	903	907	909	rVB2	41564	49754	1.50%	0.194%
23	12.797	935	937	938	rBV	39915	38456	1.16%	0.150%
24	12.819	938	939	940	rBV	52386	40433	1.22%	0.157%
25	12.991	952	954	957	rBV	2322399	3256446	98.09%	12.684%
26	13.528	999	1001	1003	rBV	31718	35642	1.07%	0.139%
27	13.882	1030	1032	1041	rBV	139802	217857	6.56%	0.849%
28	14.042	1043	1046	1048	rBV	830642	772799	23.28%	3.010%
29	15.483	1169	1172	1175	rBV	404067	529843	15.96%	2.064%

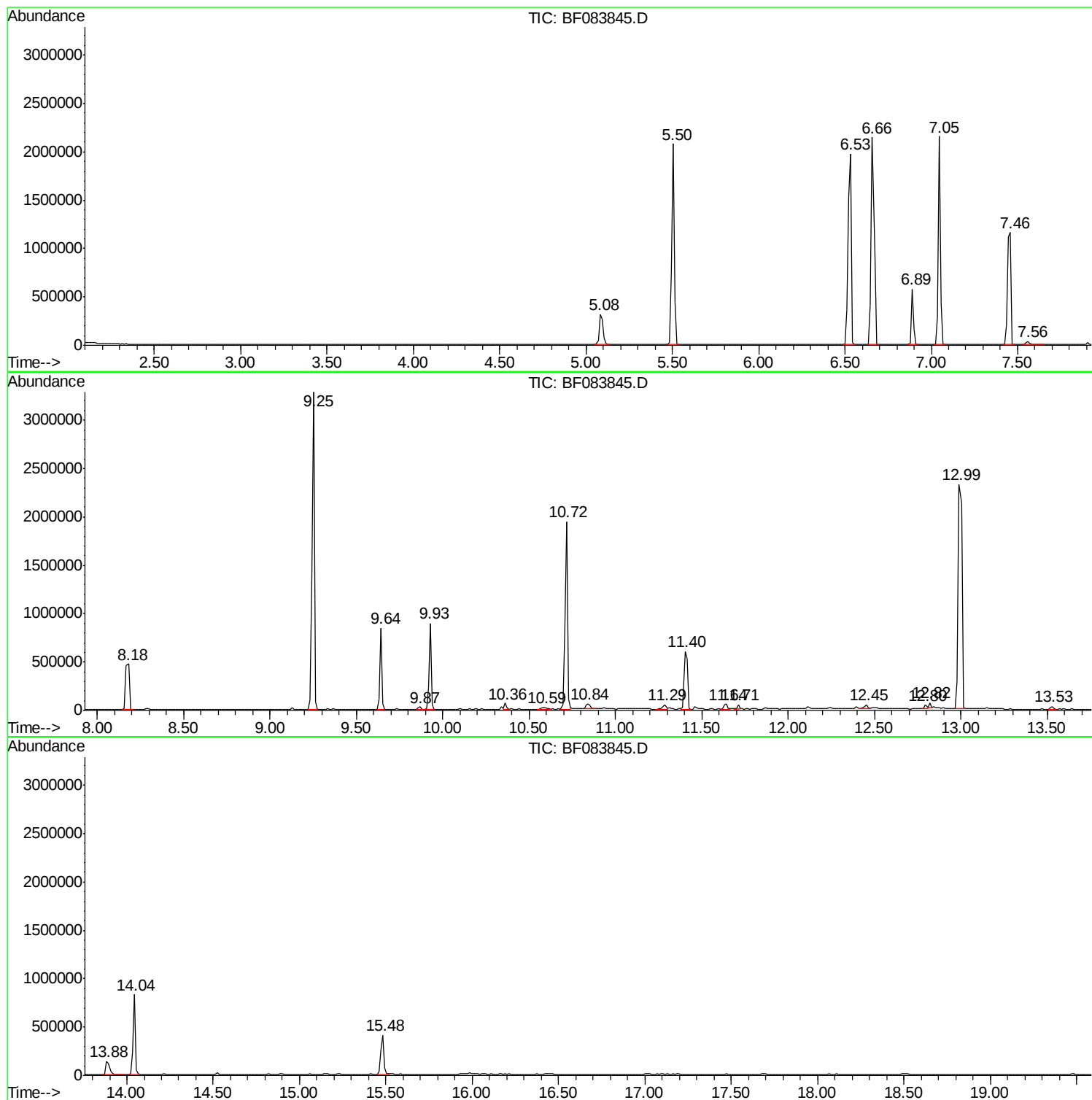
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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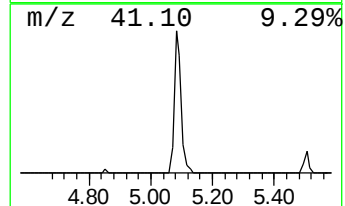
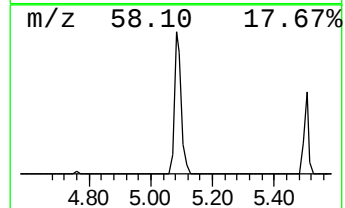
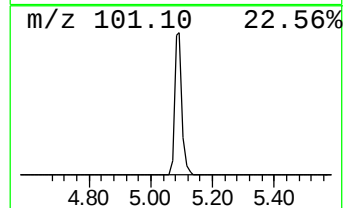
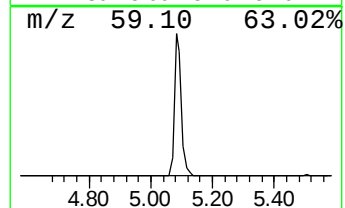
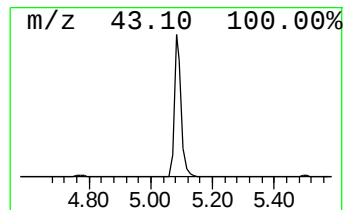
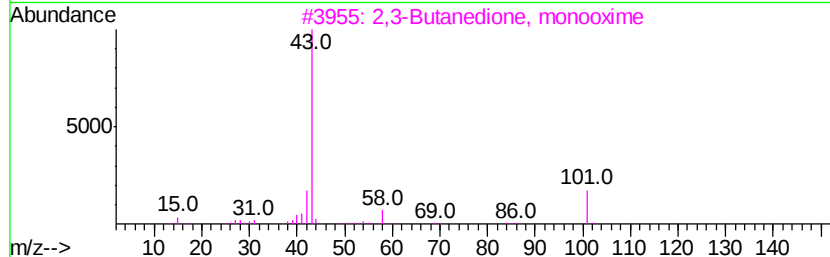
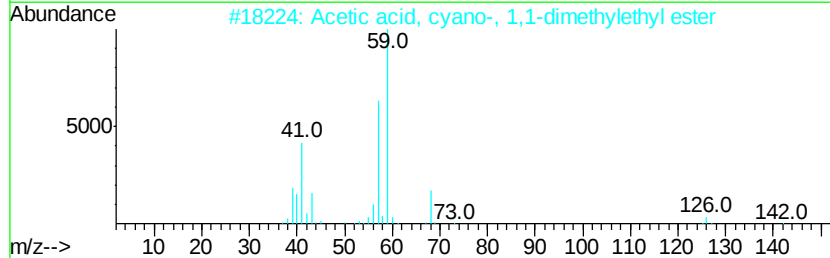
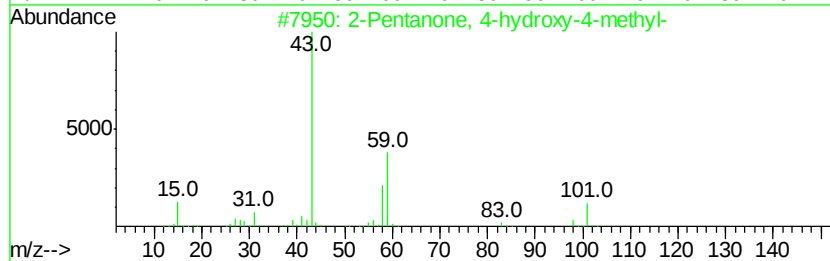
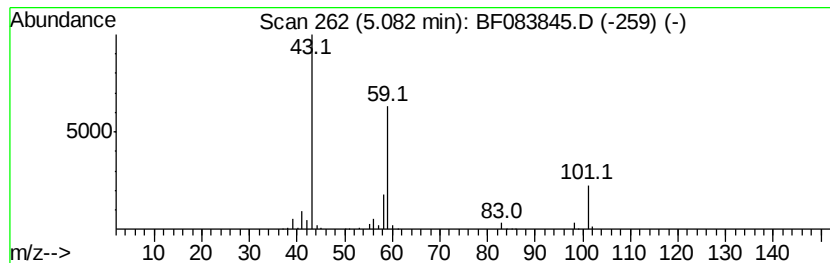
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.08	18.90 ng	486435	1,4-Dichlorobenzene-d4	6.89

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	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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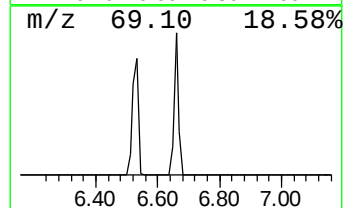
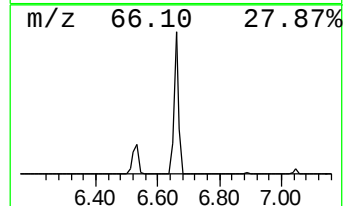
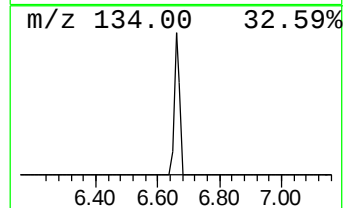
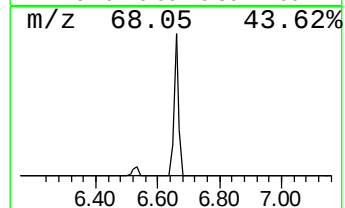
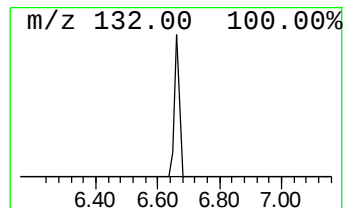
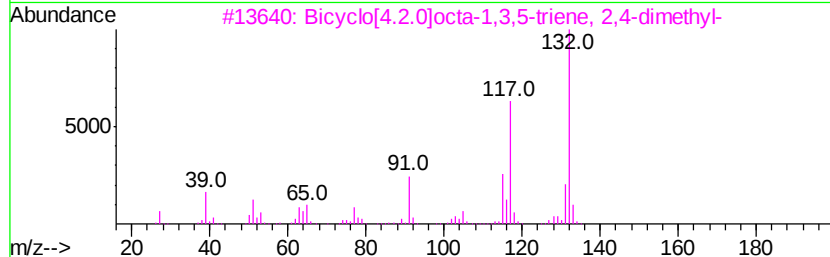
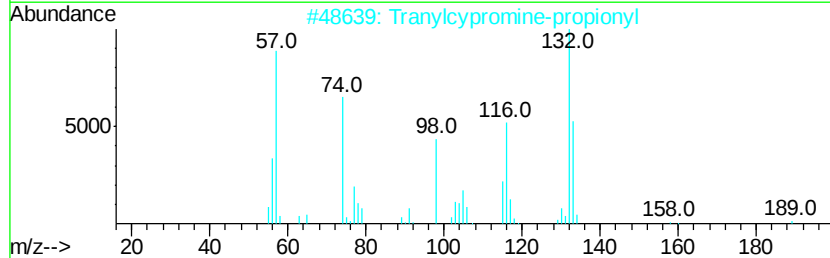
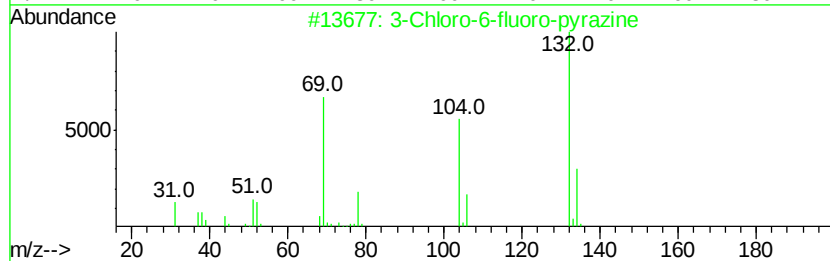
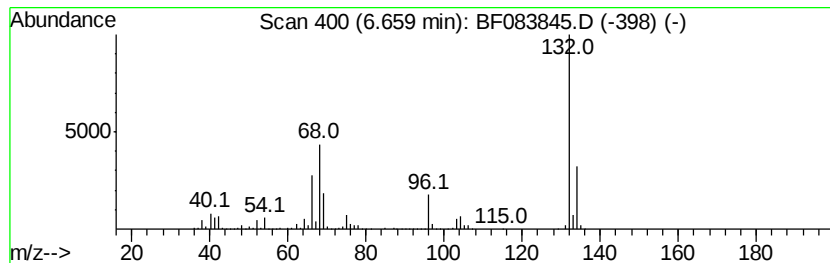
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	94.09 ng	2422070	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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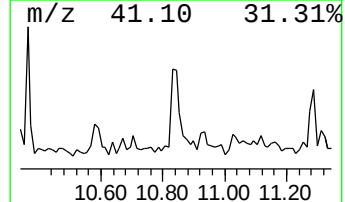
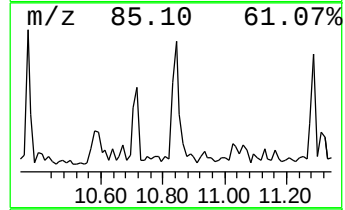
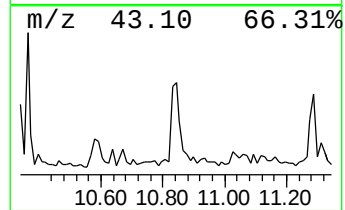
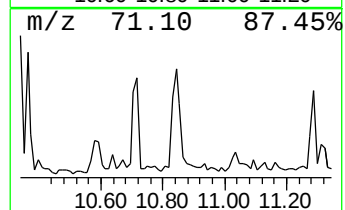
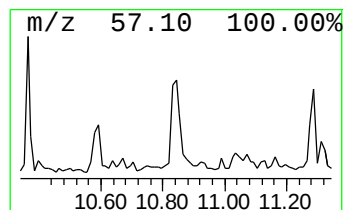
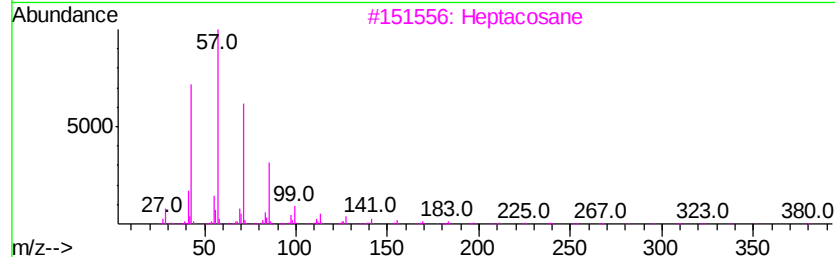
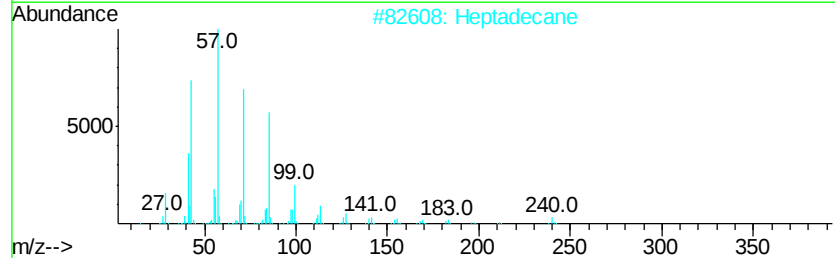
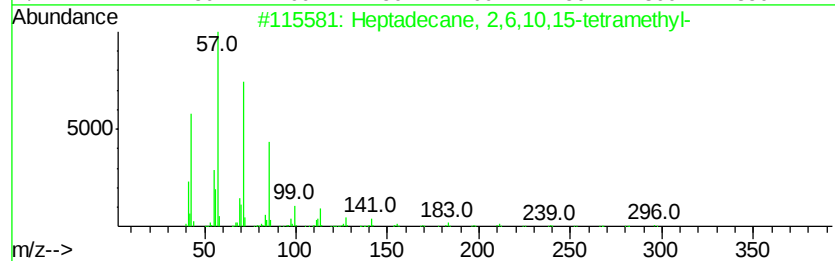
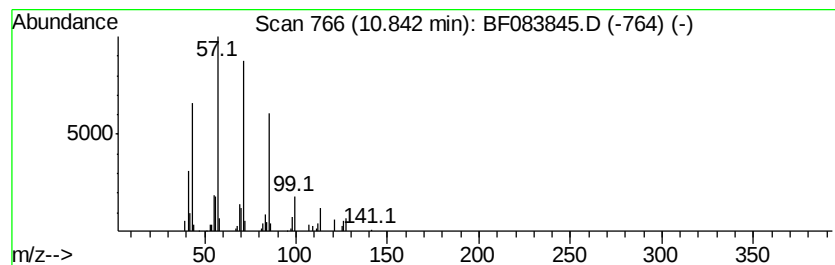
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Peak Number 4 Heptadecane, 2,6,10,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.21 ng	85450	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44		054833-48-6	86
2	Heptadecane	240	C17H36		000629-78-7	72
3	Heptacosane	380	C27H56		000593-49-7	64
4	Decane, 2,4,6-trimethyl-	184	C13H28		062108-27-4	64
5	Eicosane	282	C20H42		000112-95-8	64



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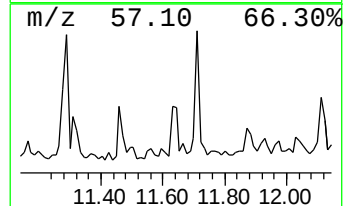
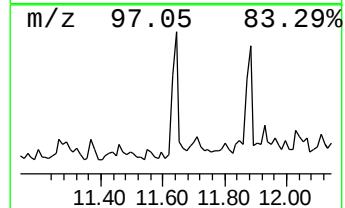
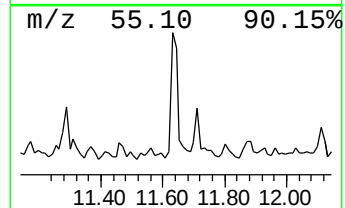
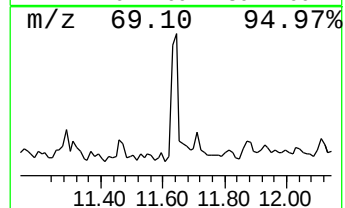
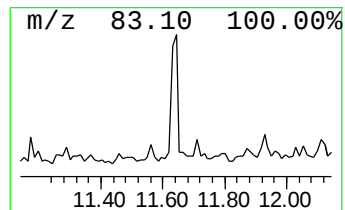
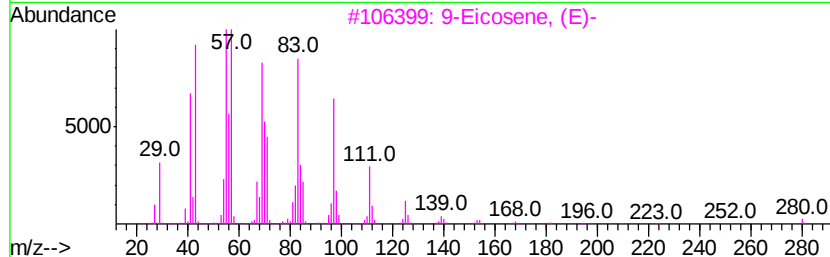
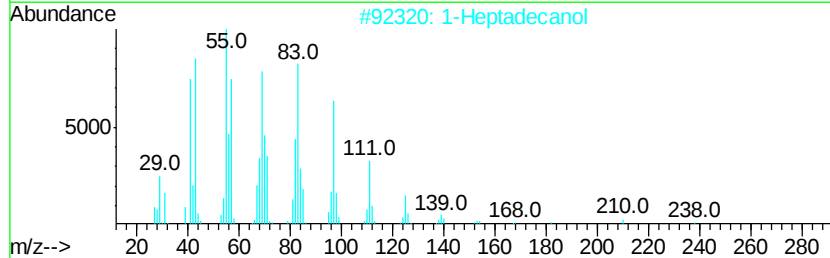
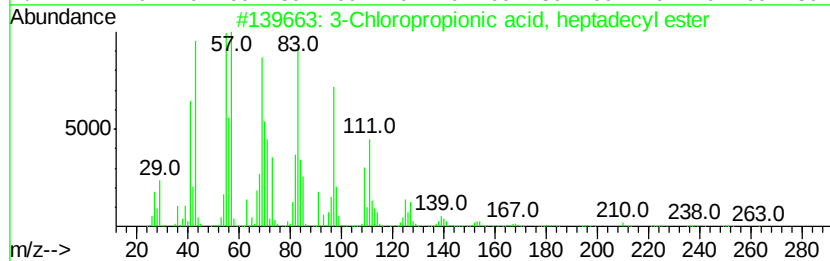
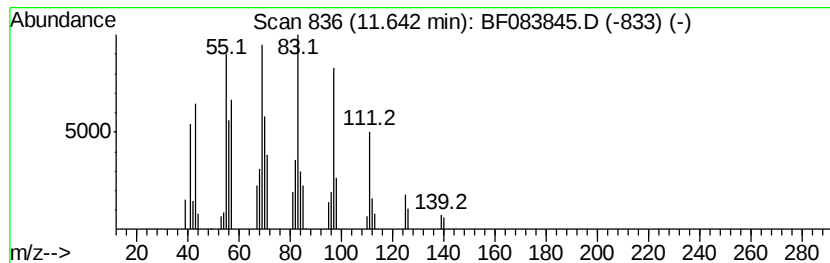
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Peak Number 5 3-Chloropropionic acid, hep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	2.06 ng	79433	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
2		1-Heptadecanol	256	C17H36O	001454-85-9	91
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4		1-Hexadecanol	242	C16H34O	036653-82-4	91
5		5-Octadecene, (E)-	252	C18H36	007206-21-5	87



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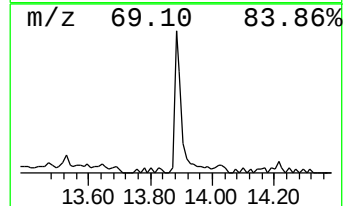
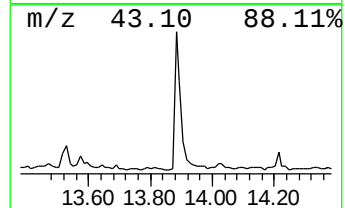
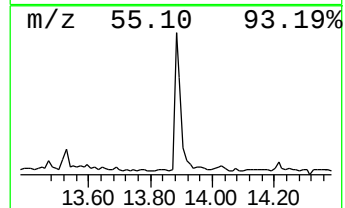
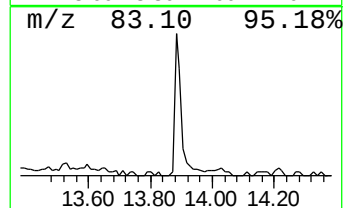
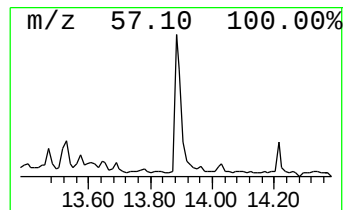
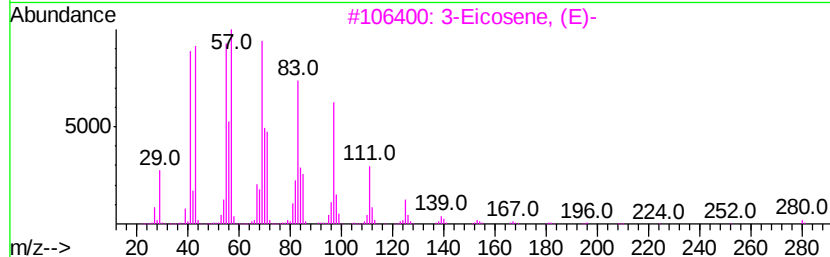
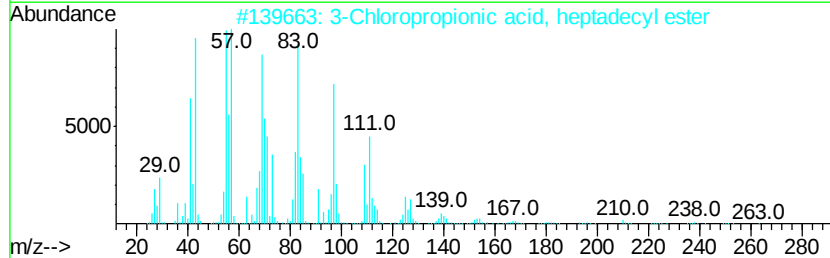
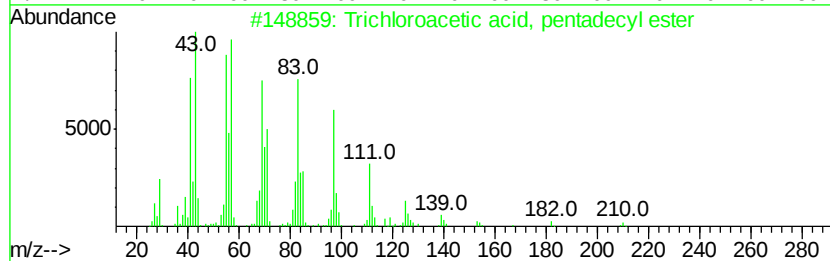
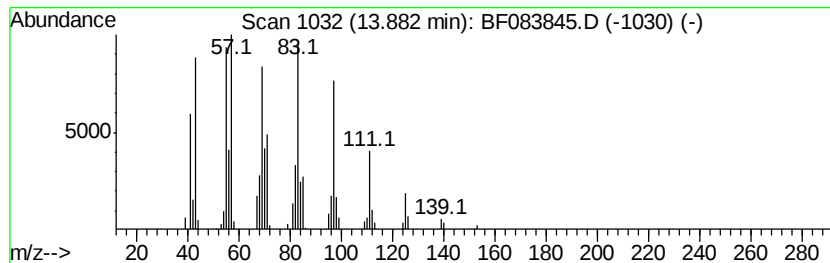
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	5.64 ng	217857	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4		5-Eicosene, (E)-	280	C20H40	074685-30-6	81
5		1-Nonadecene	266	C19H38	018435-45-5	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	18.9	ng	486435	1	6.89	514847	20.0
unknown6.66	6.66	94.1	ng	2422070	1	6.89	514847	20.0
Heptadecane, 2,6,...	10.84	2.2	ng	85450	4	11.41	772437	20.0
3-Chloropropionic...	11.64	2.1	ng	79433	4	11.41	772437	20.0
Trichloroacetic a...	13.88	5.6	ng	217857	5	14.04	772799	20.0