

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
 Data File : BF095850.D
 Acq On : 10 Jun 2017 16:26
 Operator : SJ/MA
 Sample : I3615-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HA4-WCB

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-BF060517.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	4.587	506	510	529	rBV	55454	168709	7.99%	1.009%
2	5.263	621	625	661	rBV	981540	1777045	84.13%	10.633%
3	6.928	903	908	920	rBV	1089778	1702393	80.59%	10.186%
4	7.022	920	924	941	rVB	1329381	1990476	94.23%	11.910%
5	7.369	978	983	997	rBV	232004	318165	15.06%	1.904%
6	7.604	1018	1023	1038	rBV	1030326	1403465	66.44%	8.397%
7	8.281	1133	1138	1157	rBV	698215	1069395	50.63%	6.399%
8	9.398	1323	1328	1342	rBV	308282	437680	20.72%	2.619%
9	11.180	1624	1631	1648	rBV	1504377	2112286	100.00%	12.639%
10	11.875	1744	1749	1763	rBV	263442	358971	16.99%	2.148%
11	12.222	1802	1808	1824	rVB2	358582	508625	24.08%	3.043%
12	13.516	2023	2028	2042	rBV	726887	1022774	48.42%	6.120%
13	13.845	2080	2084	2094	rBV2	13881	22291	1.06%	0.133%
14	14.616	2211	2215	2226	rVB	373847	508961	24.10%	3.045%
15	15.316	2328	2334	2342	rVB2	10780	21946	1.04%	0.131%
16	15.627	2379	2387	2395	rBV2	15828	33383	1.58%	0.200%
17	16.733	2568	2575	2586	rBV3	24552	51826	2.45%	0.310%
18	16.992	2613	2619	2623	rBV2	1631201	2103615	99.59%	12.587%
19	18.245	2828	2832	2842	rBV	113081	176785	8.37%	1.058%
20	18.333	2842	2847	2858	rVV	417587	513629	24.32%	3.073%
21	20.003	3126	3131	3141	rBV	255850	369954	17.51%	2.214%
22	20.492	3209	3214	3218	rBV6	24203	40598	1.92%	0.243%

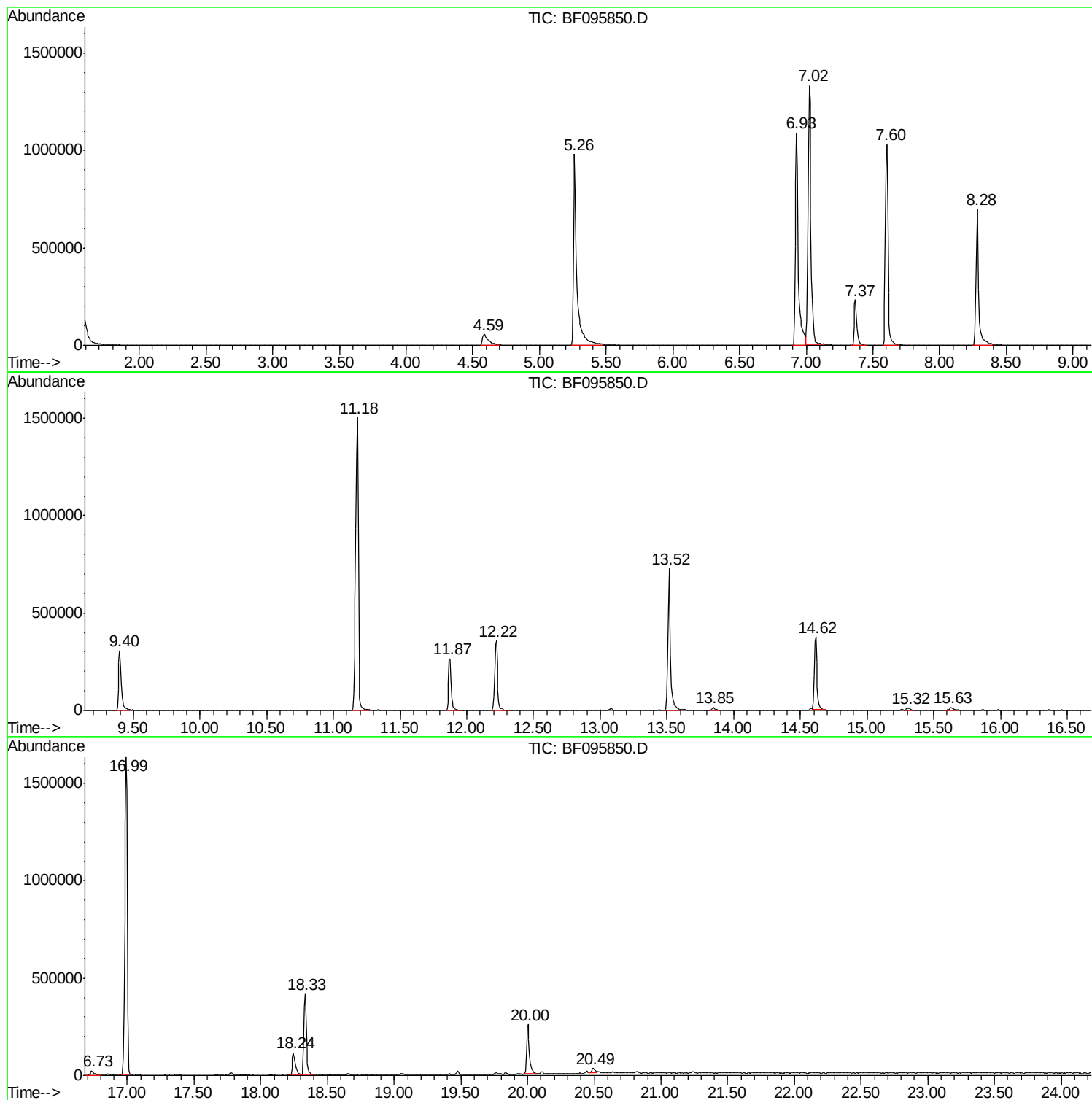
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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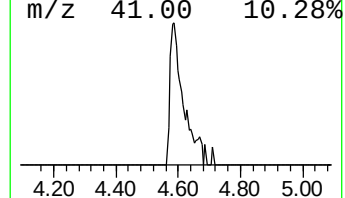
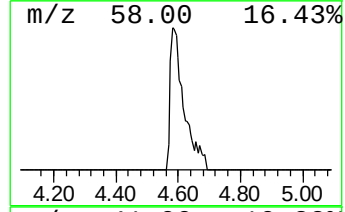
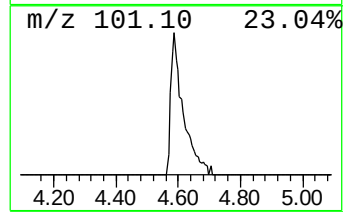
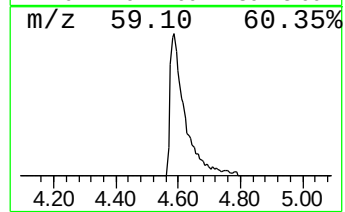
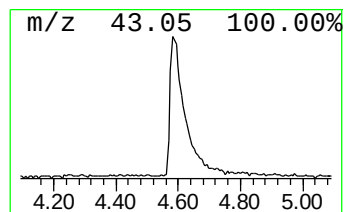
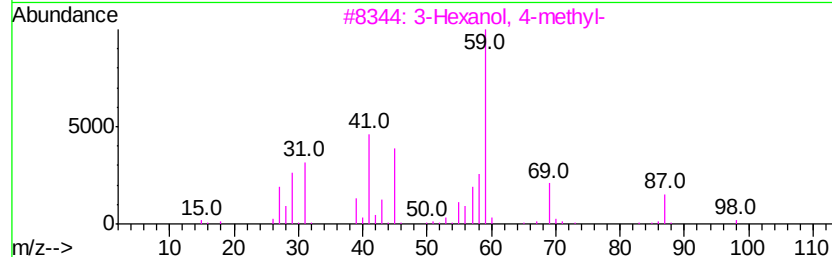
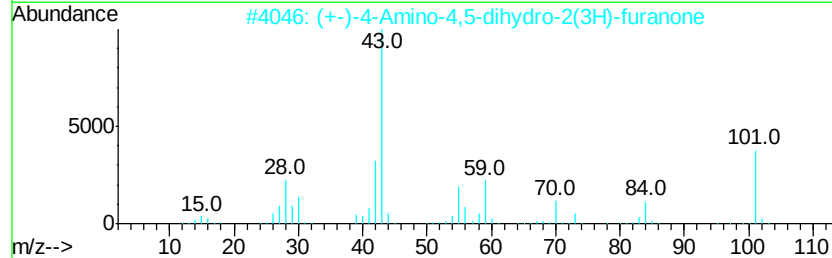
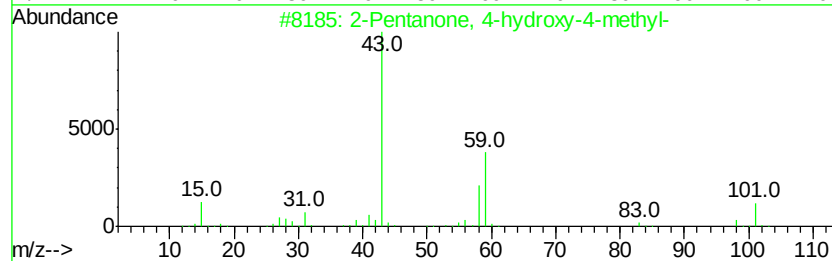
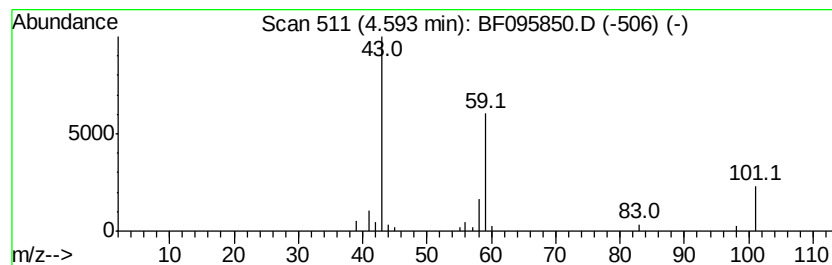
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	10.61 ng	168709	1,4-Dichlorobenzene-d4	7.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	47
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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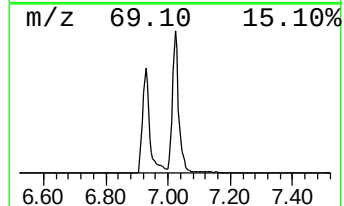
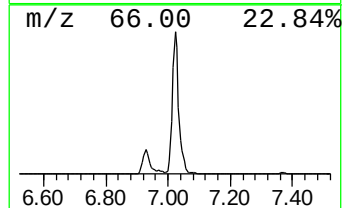
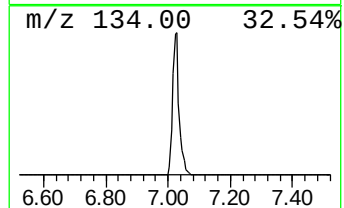
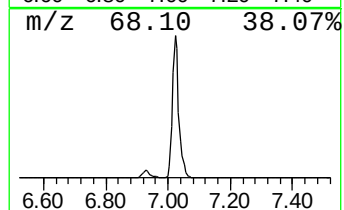
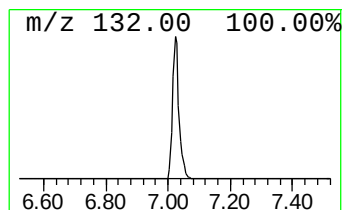
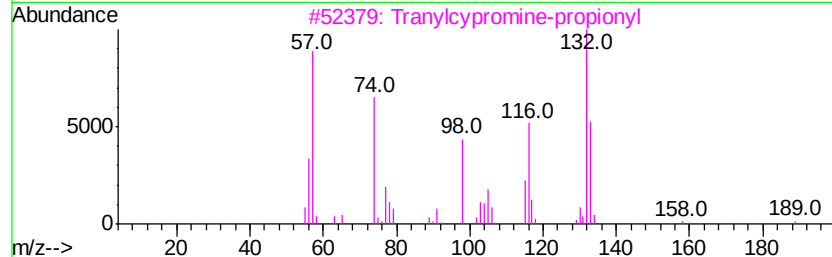
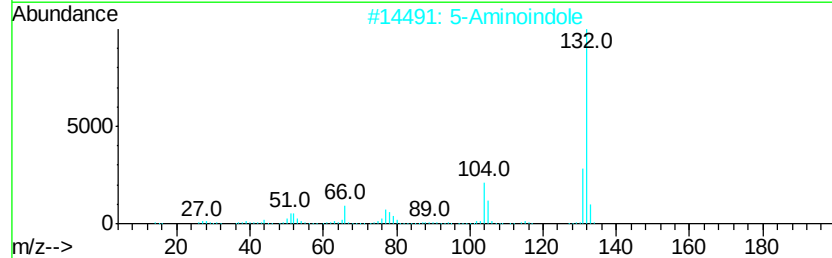
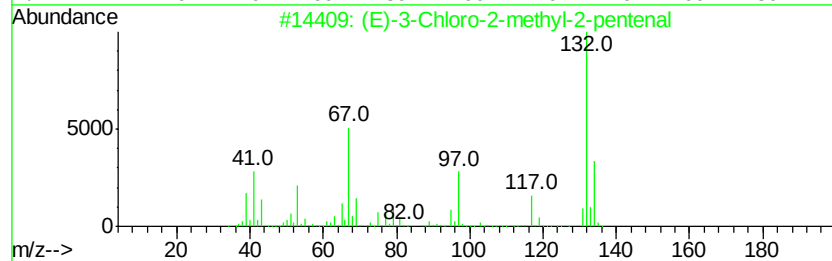
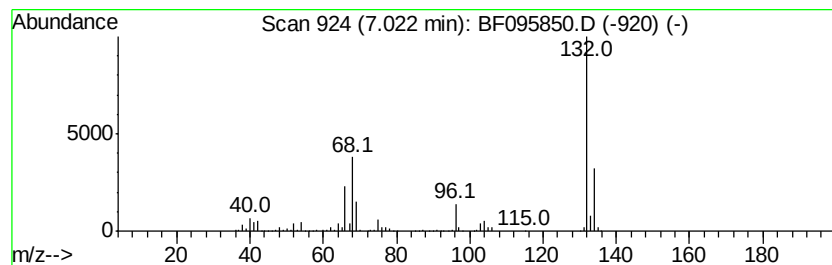
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Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	125.12 ng	1990480	1,4-Dichlorobenzene-d4	7.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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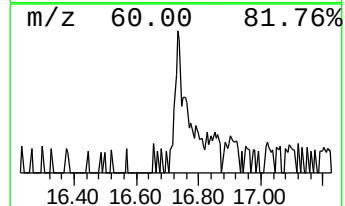
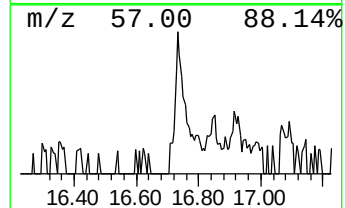
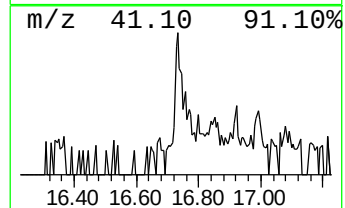
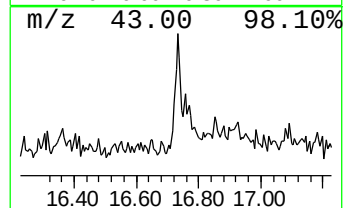
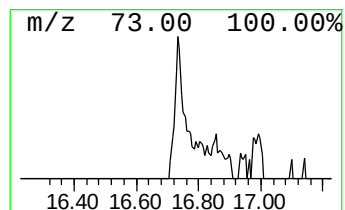
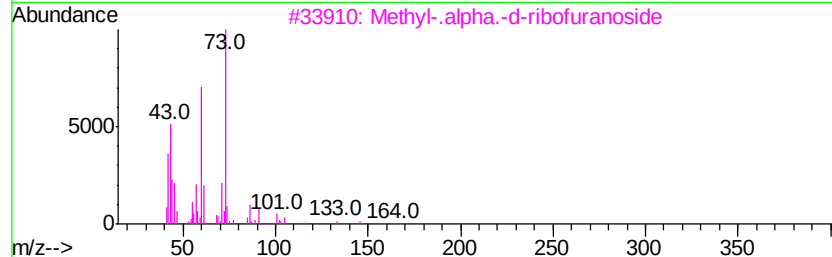
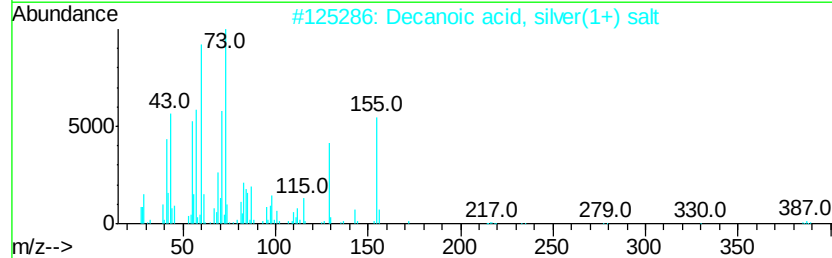
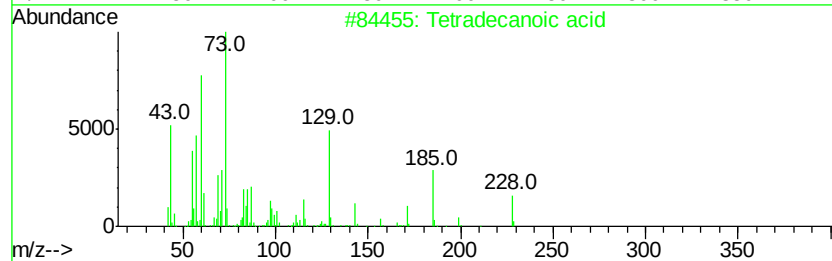
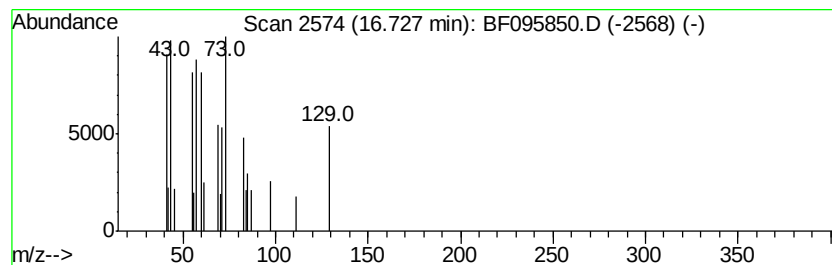
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Peak Number 4 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.02 ng	51826	Chrysene-d12	18.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecanoic acid	228 C14H28O2	000544-63-8 64
2		Decanoic acid, silver(1+) salt	278 C10H19AgO2	013126-67-5 64
3		Methyl-.alpha.-d-ribofuranoside	164 C6H12O5	1000129-83-1 35
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129 C5H7NOS	029926-41-8 35
5		Isoamyl nitrite	117 C5H11NO2	000110-46-3 27



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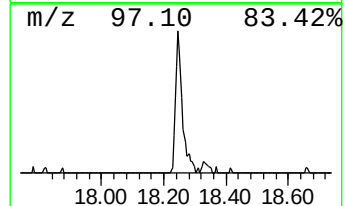
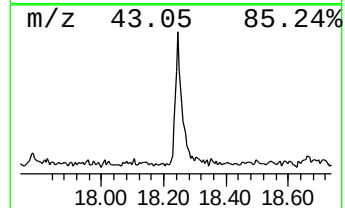
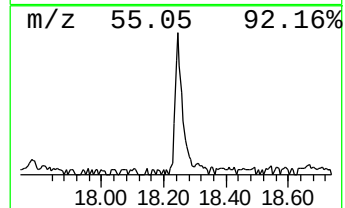
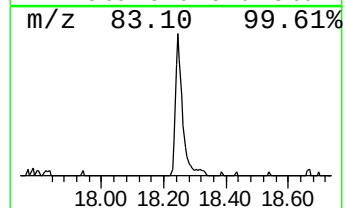
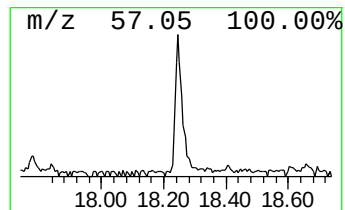
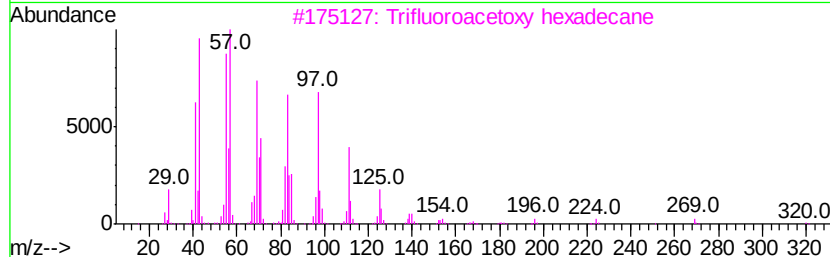
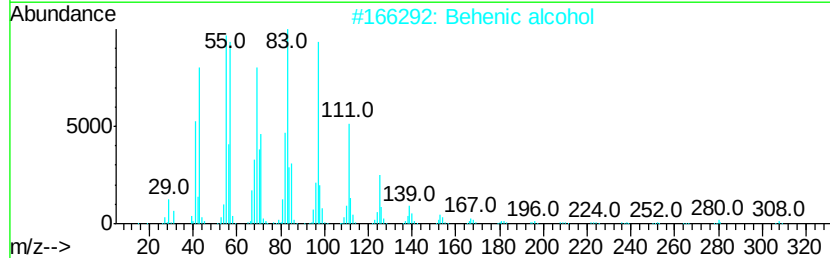
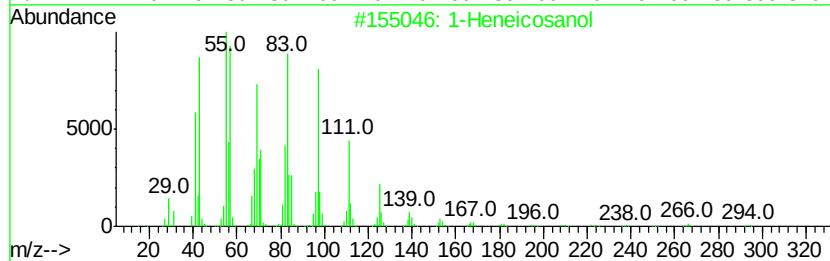
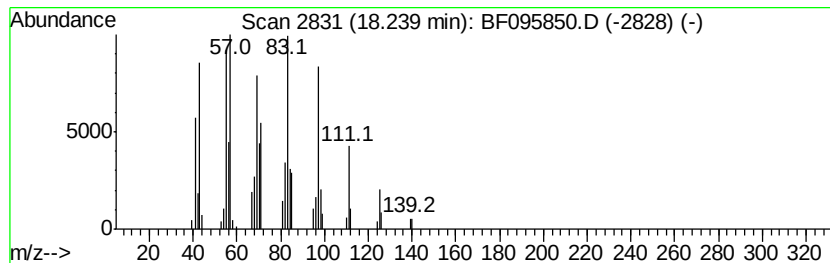
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.24	6.88 ng	176785	Chrysene-d12	18.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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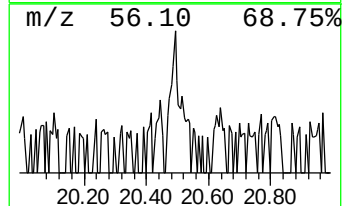
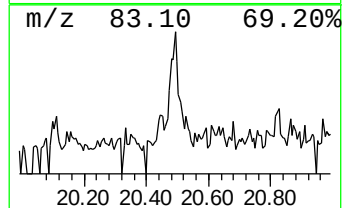
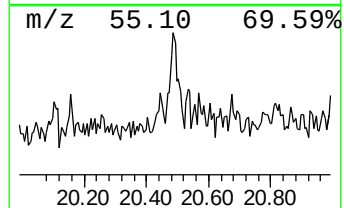
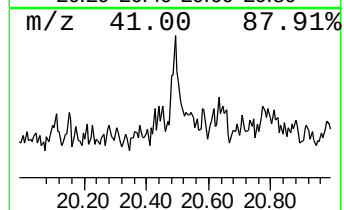
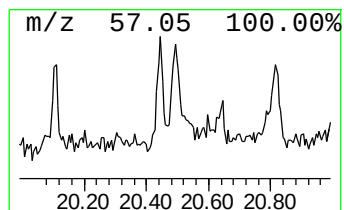
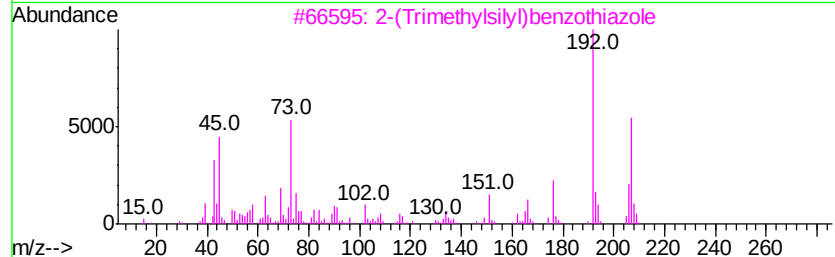
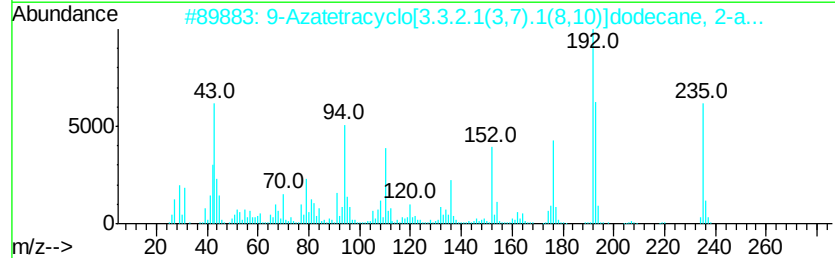
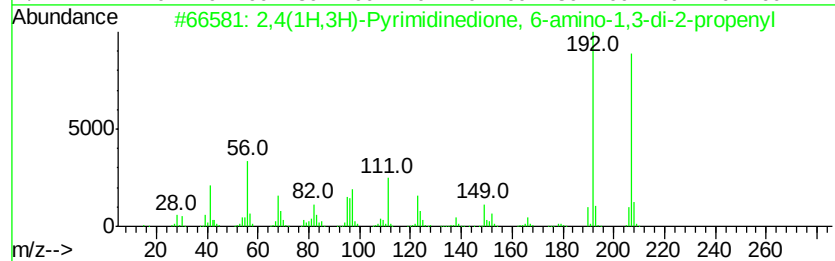
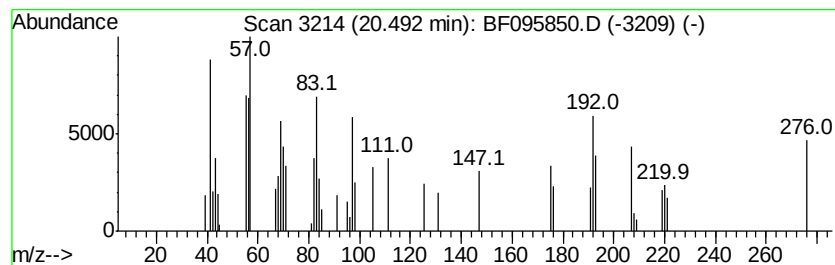
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Peak Number 6 unknown20.49 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.49	2.19 ng	40598	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4(1H,3H)-Pvrimidinedione, 6-am...	207	C10H13N3O2	004852-19-1	22
2		9-Azatetracyclo[3.3.2.1(3,7).1(8...	235	C14H21N02	1000193-20-4	22
3		2-(Trimethylsilyl)benzothiazole	207	C10H13NSSi	032137-73-8	22
4		4H-Pyrido[1,2-a]pyrimidin-4-one,...	207	C10H13N3O2	1000337-72-2	18
5		(p-Nitrobenzoyl)acetone	207	C10H9N04	004023-82-9	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.59	10.6	ng	168709	1	7.37	318165	20.0
unknown7.02	7.02	125.1	ng	1990480	1	7.37	318165	20.0
Tetradecanoic acid	16.73	2.0	ng	51826	5	18.33	513629	20.0
1-Heneicosanol	18.24	6.9	ng	176785	5	18.33	513629	20.0
unknown20.49	20.49	2.2	ng	40598	6	20.00	369954	20.0