

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103117\
 Data File : BF100011.D
 Acq On : 31 Oct 2017 18:51
 Operator : SJ/JU
 Sample : I6213-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-019

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	5.004	493	496	522	rBV	147741	245855	13.19%	1.487%
2	5.410	562	565	595	rBV	1313885	1523440	81.76%	9.213%
3	6.434	735	739	757	rBV	1457306	1539576	82.63%	9.311%
4	6.557	757	760	776	rVB	1697148	1645725	88.32%	9.953%
5	6.787	796	799	814	rVB	606008	535669	28.75%	3.240%
6	6.940	822	825	843	rBV	1461225	1263202	67.79%	7.639%
7	7.357	893	896	914	rBV	1055502	970208	52.07%	5.868%
8	8.069	1014	1017	1030	rBV	909474	748793	40.19%	4.528%
9	8.634	1109	1113	1119	rBB	22071	22323	1.20%	0.135%
10	9.145	1196	1200	1203	rBV	2089397	1863317	100.00%	11.269%
11	9.539	1264	1267	1279	rBV	609863	516553	27.72%	3.124%
12	9.822	1312	1315	1326	rVB	854545	820002	44.01%	4.959%
13	10.539	1434	1437	1448	rVB	89720	75305	4.04%	0.455%
14	10.622	1448	1451	1465	rBV	1039880	1010811	54.25%	6.113%
15	11.322	1566	1570	1579	rBV	824208	781439	41.94%	4.726%
16	11.833	1654	1657	1661	rBV	65718	64468	3.46%	0.390%
17	12.621	1788	1791	1803	rBV2	26880	41098	2.21%	0.249%
18	12.786	1816	1819	1822	rVB	25271	21620	1.16%	0.131%
19	12.904	1835	1839	1842	rBV	1718995	1516978	81.41%	9.174%
20	13.786	1985	1989	1995	rBV	68279	84001	4.51%	0.508%
21	13.980	2018	2022	2031	rBV	485290	543820	29.19%	3.289%
22	14.421	2094	2097	2105	rVB8	18165	31655	1.70%	0.191%
23	15.057	2202	2205	2209	rVB2	33218	33547	1.80%	0.203%
24	15.468	2270	2275	2285	rBV	346327	487728	26.18%	2.950%
25	15.633	2298	2303	2307	rBV8	17092	30776	1.65%	0.186%
26	15.910	2346	2350	2358	rVB3	23765	37492	2.01%	0.227%
27	17.421	2602	2607	2618	rBV3	27493	79813	4.28%	0.483%

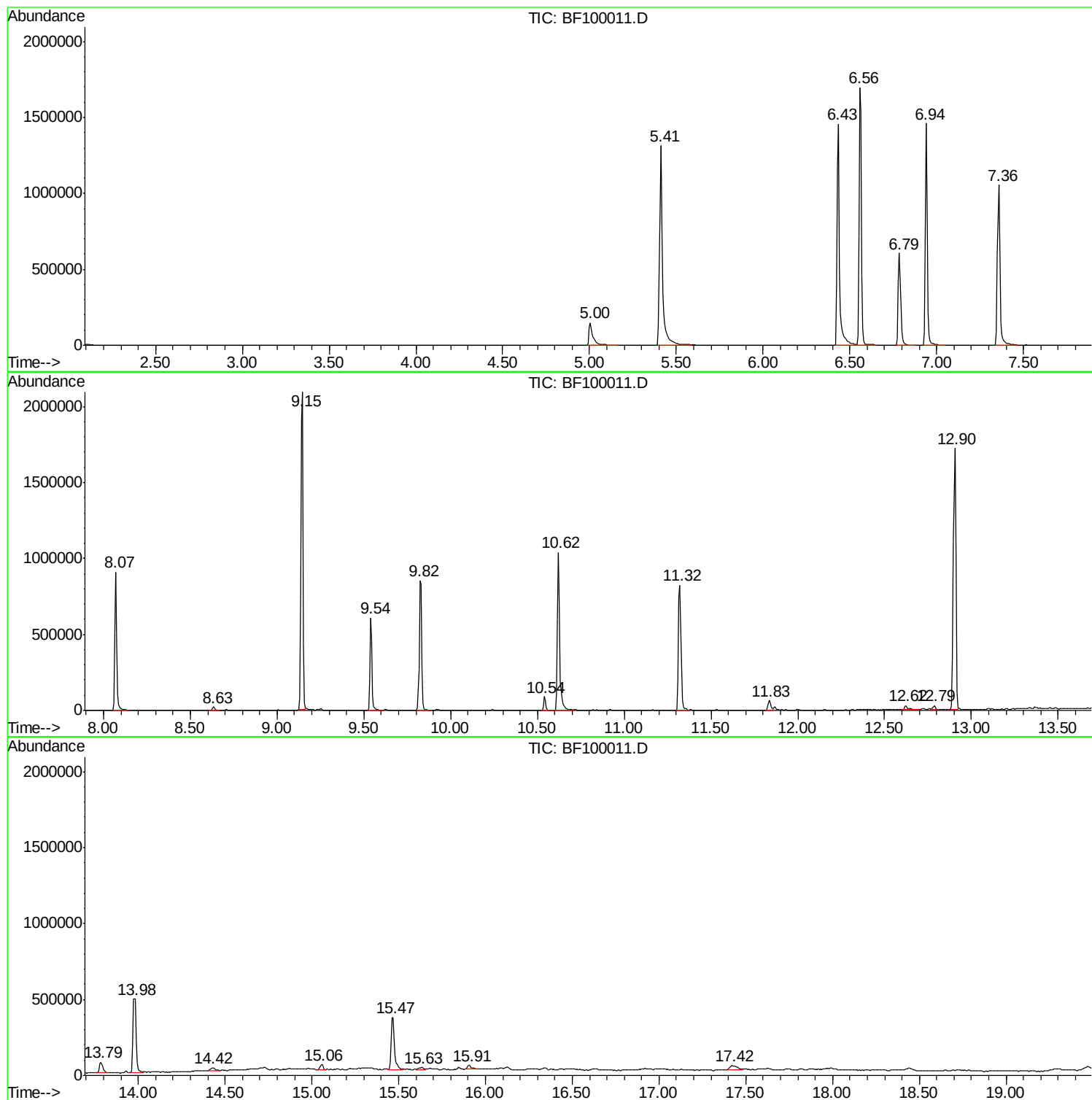
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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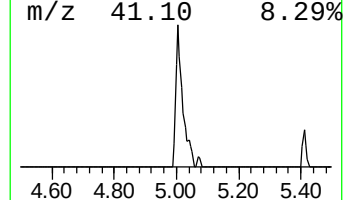
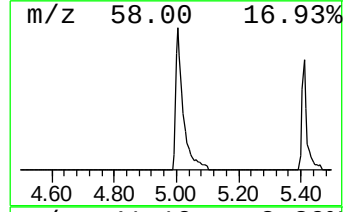
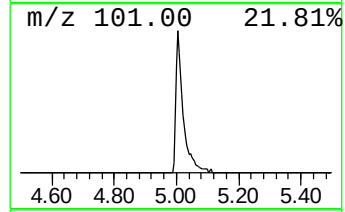
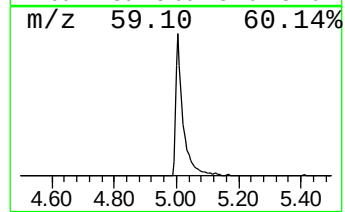
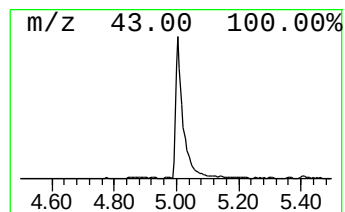
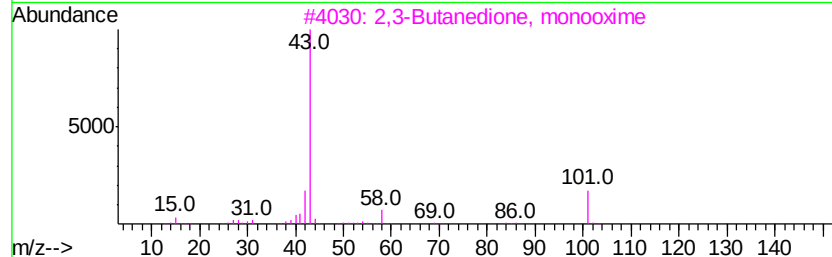
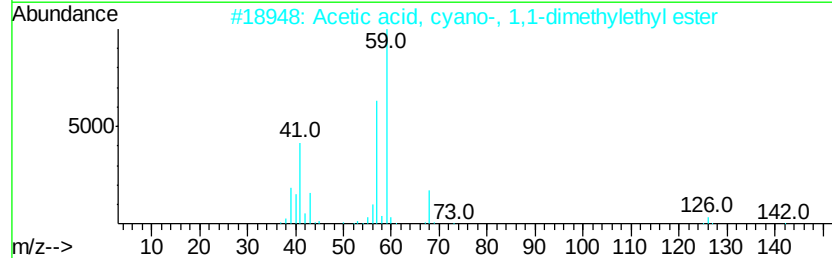
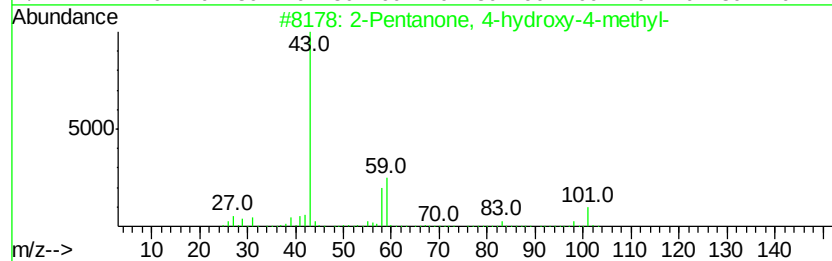
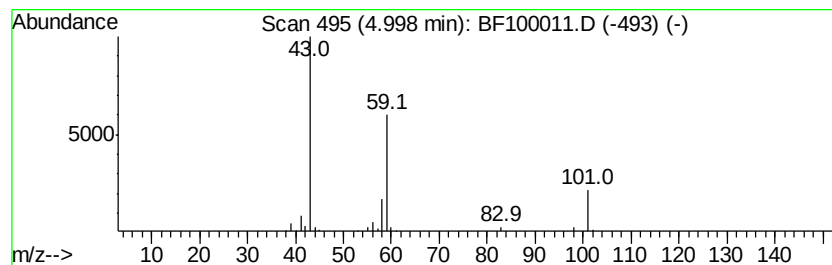
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
5.00	9.18 ng	245855	1,4-Dichlorobenzene-d4	6.79

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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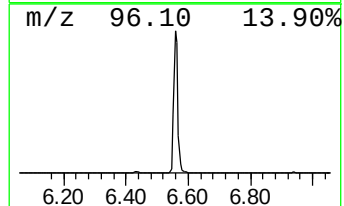
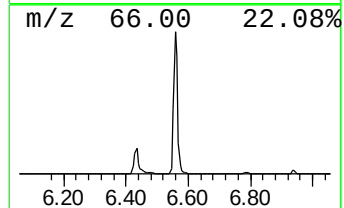
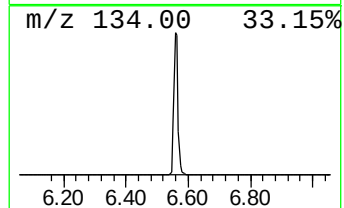
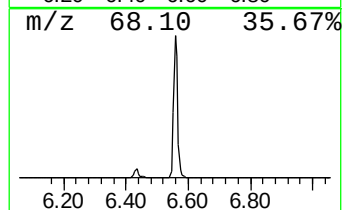
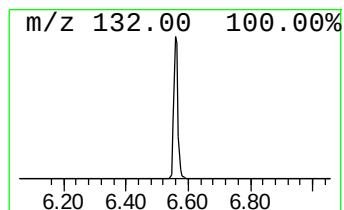
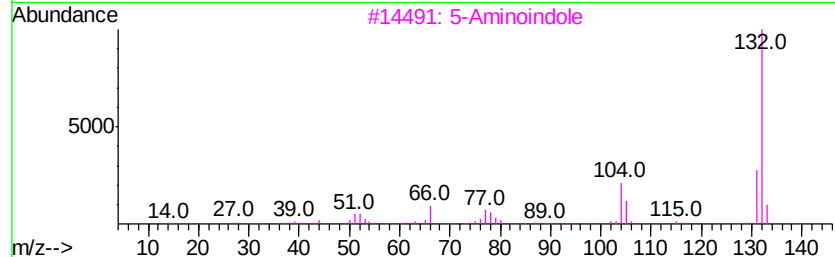
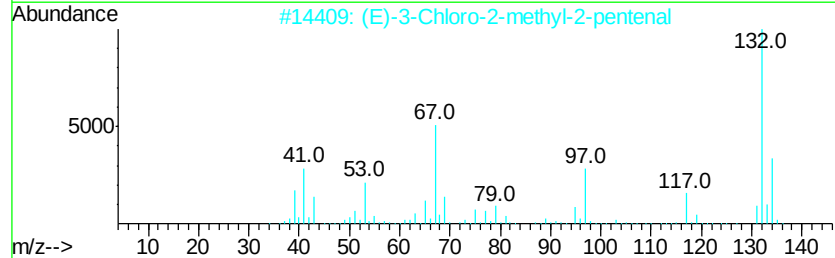
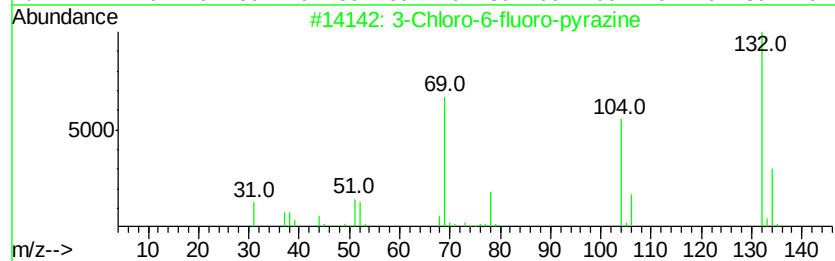
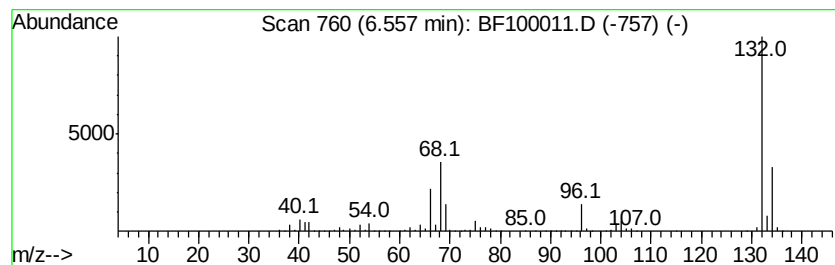
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	61.45 ng	1645730	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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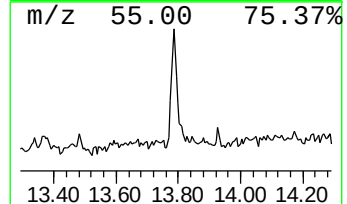
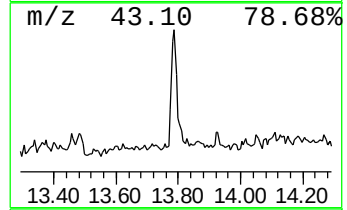
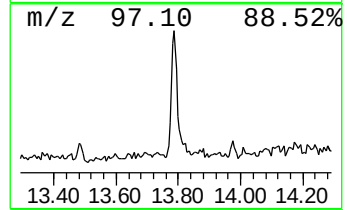
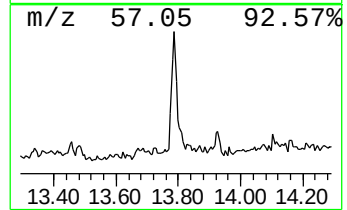
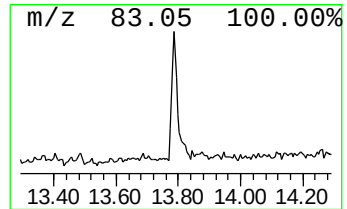
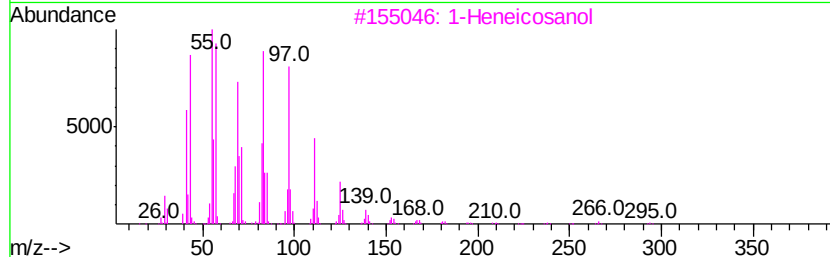
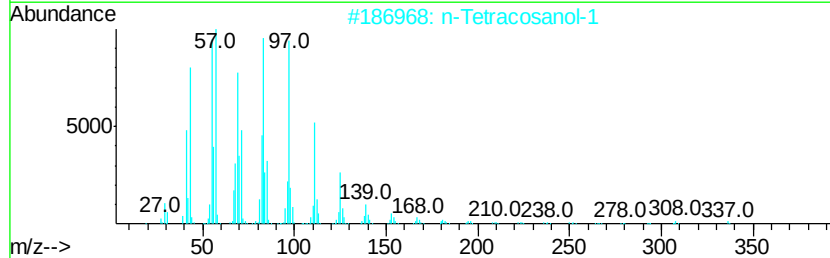
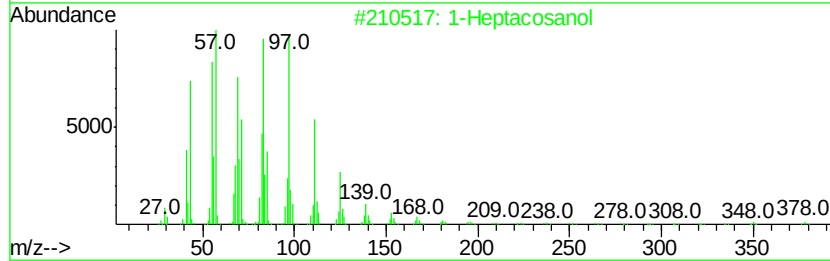
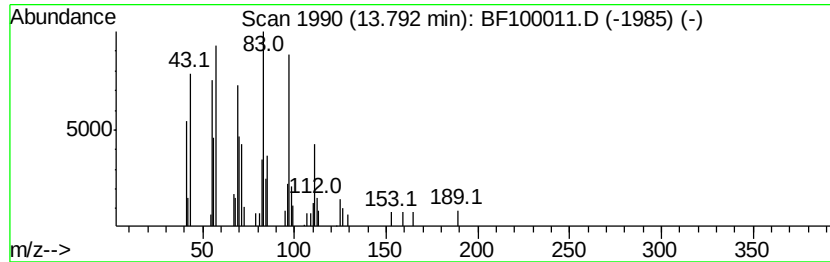
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Peak Number 4 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.79	3.09 ng	84001	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	81



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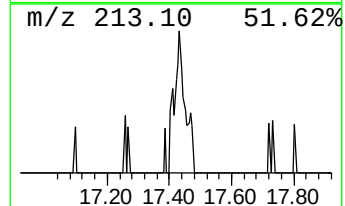
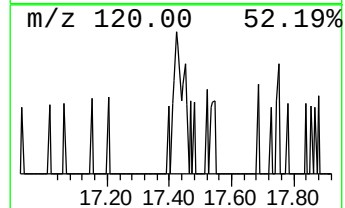
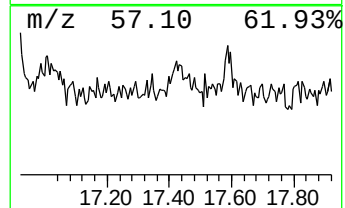
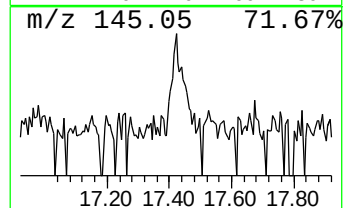
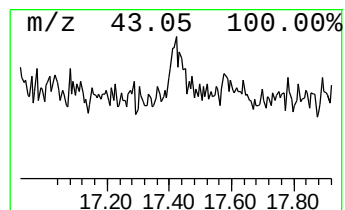
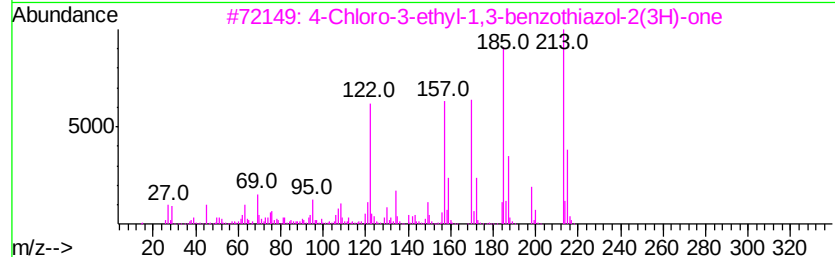
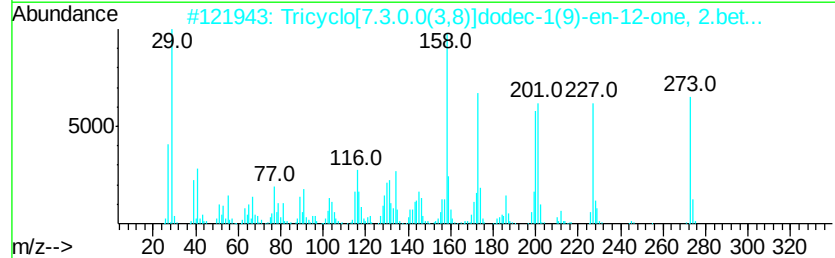
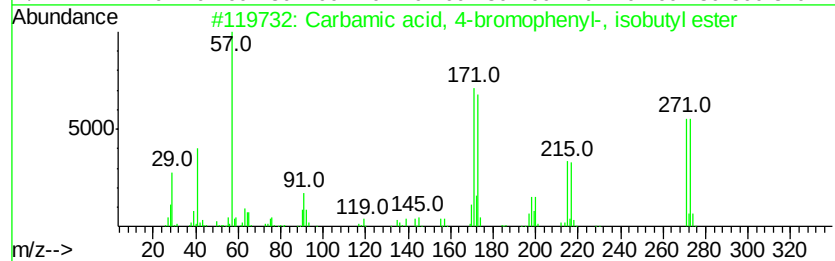
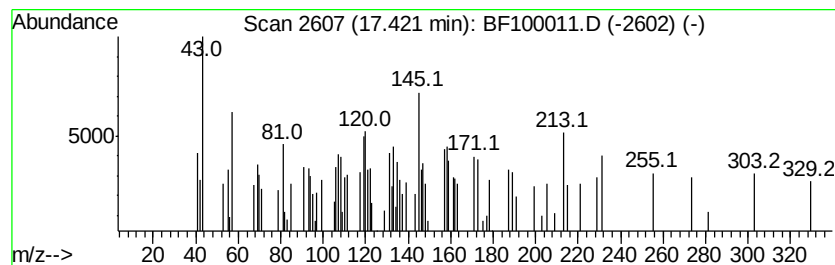
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Peak Number 5 unknown17.42 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	3.27 ng	79813	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbamic acid, 4-bromophenyl-, i...	271	C11H14BrN02	1000314-74-4	14
2		Tricyclo[7.3.0.0(3,8)]dodec-1(9)...	273	C16H19N03	1000160-30-7	14
3		4-Chloro-3-ethyl-1,3-benzothiazol...	213	C9H8ClN0S	1000331-84-8	11
4		5-Pyrimidinamine, 2-chloro-4-eth...	173	C6H8ClN3O	054484-70-7	9
5		Norflurazon	303	C12H9ClF3N3O	027314-13-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	9.2	ng	245855	1	6.79	535669	20.0
unknown6.56	6.56	61.5	ng	1645730	1	6.79	535669	20.0
1-Heptacosanol	13.79	3.1	ng	84001	5	13.98	543820	20.0
unknown17.42	17.42	3.3	ng	79813	6	15.47	487728	20.0