

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
 Data File : BF098820.D
 Acq On : 26 Sep 2017 9:28
 Operator : SJ/JU
 Sample : I5384-05
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 092017-SIDI-F-U-B

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-BF092317.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	2.210	17	21	28	rVB	286328	377883	7.78%	1.365%
2	5.134	514	518	526	rVB	230484	239927	4.94%	0.867%
3	5.528	580	585	588	rBV	1596607	1417811	29.20%	5.122%
4	6.528	751	755	758	rBV	1203101	975456	20.09%	3.524%
5	6.681	776	781	784	rBV	2806625	2544566	52.40%	9.193%
6	6.910	817	820	824	rBV	940674	801040	16.50%	2.894%
7	7.069	843	847	851	rBV	3356926	3279955	67.54%	11.849%
8	7.475	910	916	919	rBV	2480526	2744030	56.51%	9.913%
9	8.192	1034	1038	1042	rBV	1302258	1090323	22.45%	3.939%
10	9.275	1216	1222	1225	rBV	4563236	4856037	100.00%	17.543%
11	9.657	1283	1287	1290	rBV	143237	103111	2.12%	0.373%
12	9.951	1333	1337	1340	rBV	1383575	1192504	24.56%	4.308%
13	10.739	1466	1471	1474	rBV	1965991	1819053	37.46%	6.572%
14	11.433	1585	1589	1593	rBV	1218258	1101176	22.68%	3.978%
15	11.992	1680	1684	1687	rVB	162406	141552	2.91%	0.511%
16	13.021	1854	1859	1862	rBV	3630293	3600779	74.15%	13.008%
17	13.904	2005	2009	2016	rBV	82569	90009	1.85%	0.325%
18	14.074	2034	2038	2041	rVB	703908	659657	13.58%	2.383%
19	15.562	2285	2291	2298	rBV	517051	645648	13.30%	2.332%

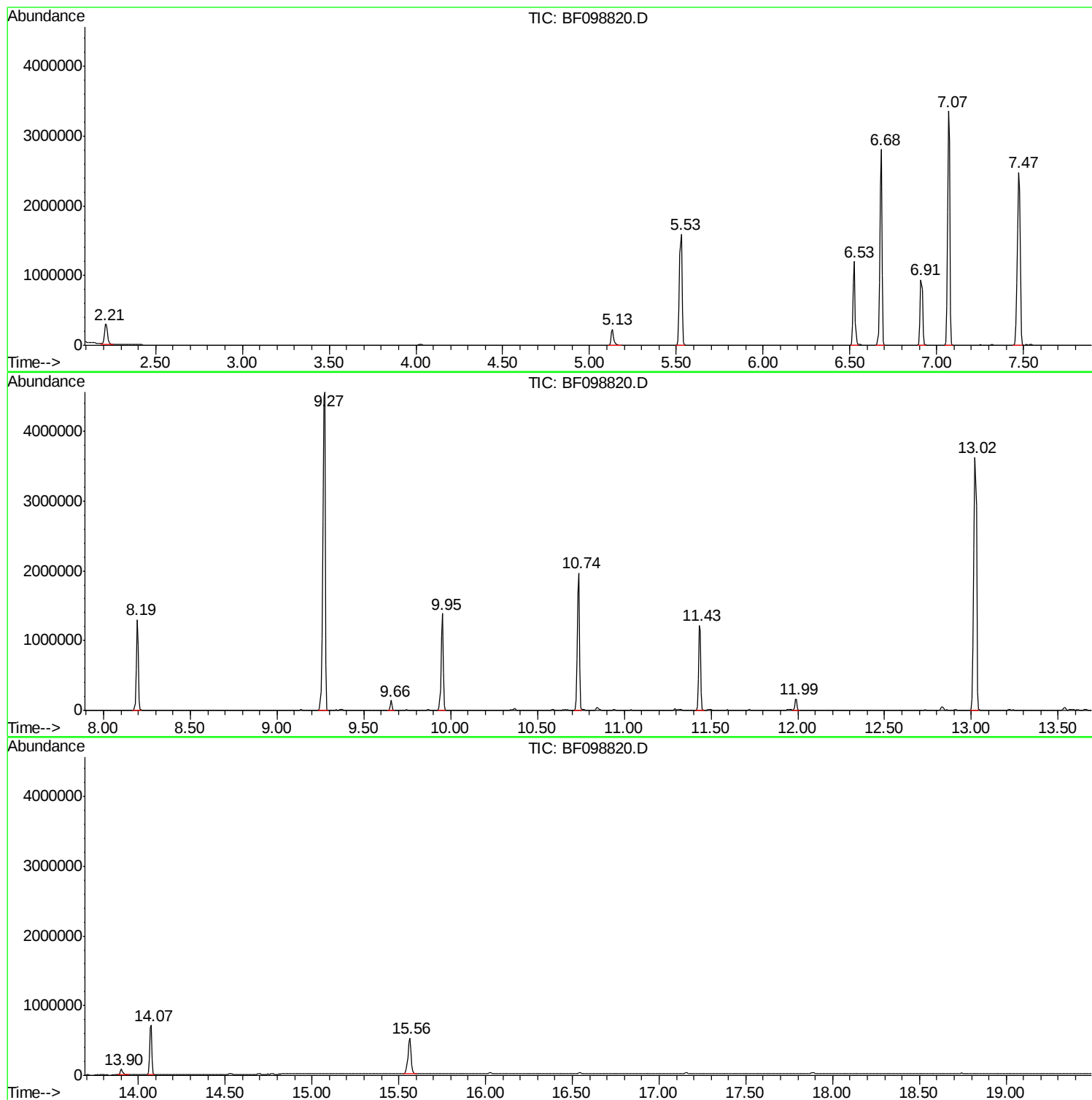
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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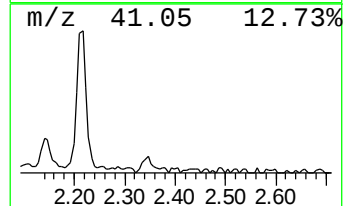
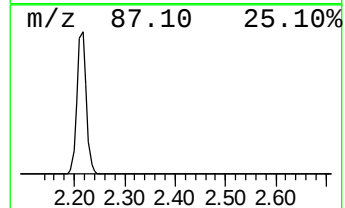
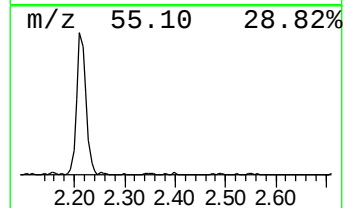
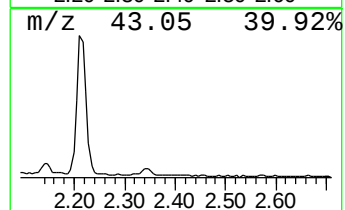
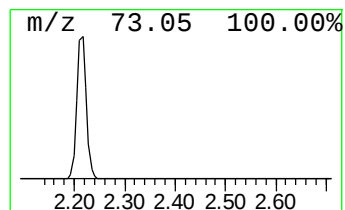
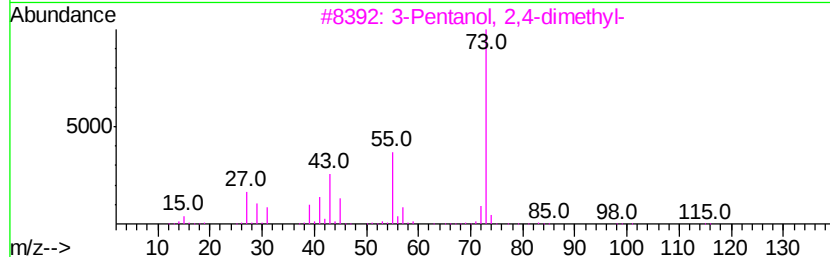
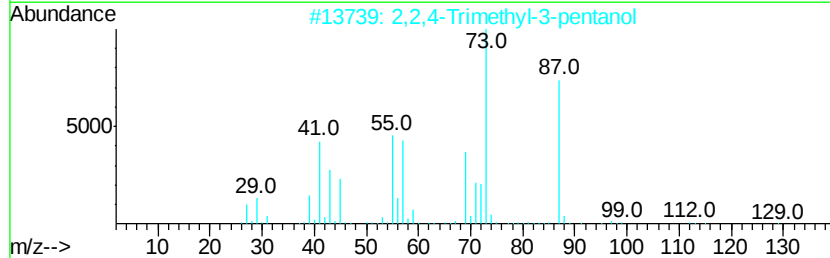
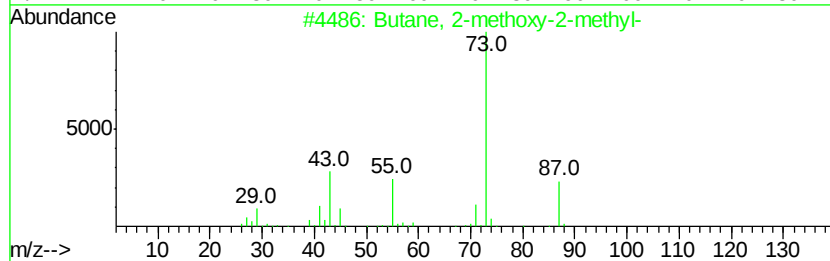
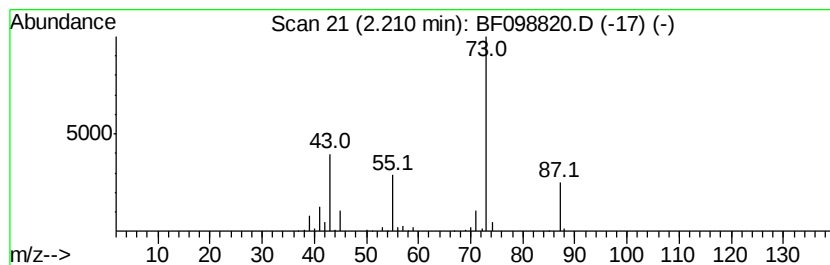
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	9.43 ng	377883	1,4-Dichlorobenzene-d4	6.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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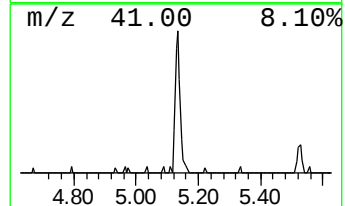
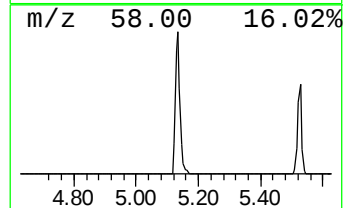
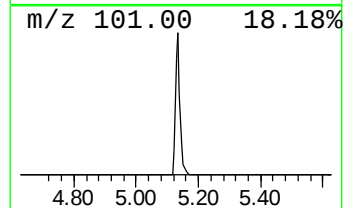
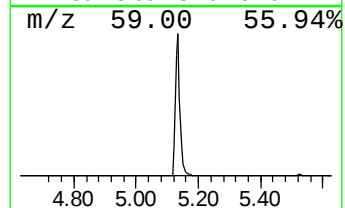
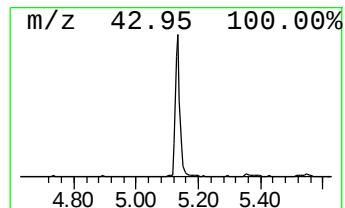
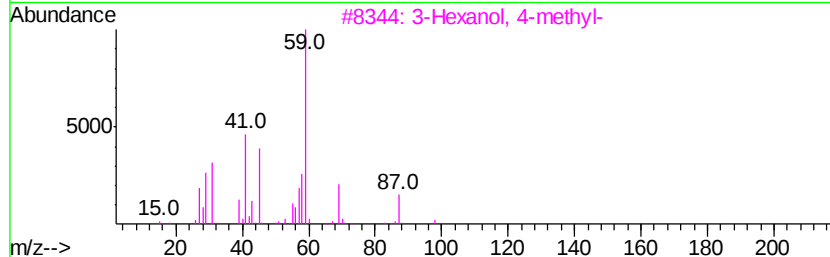
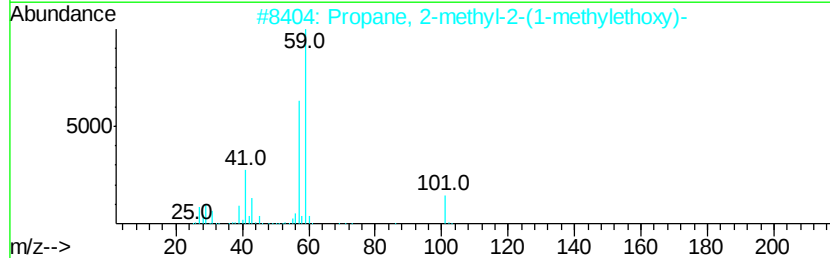
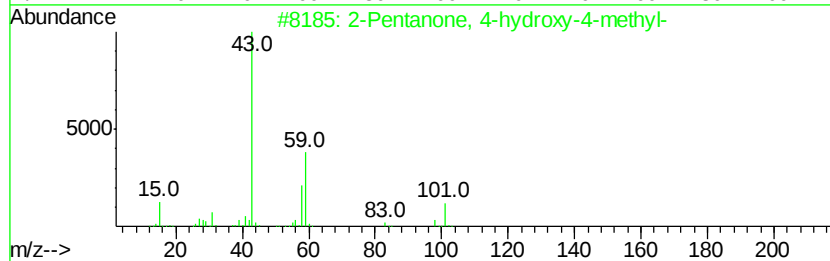
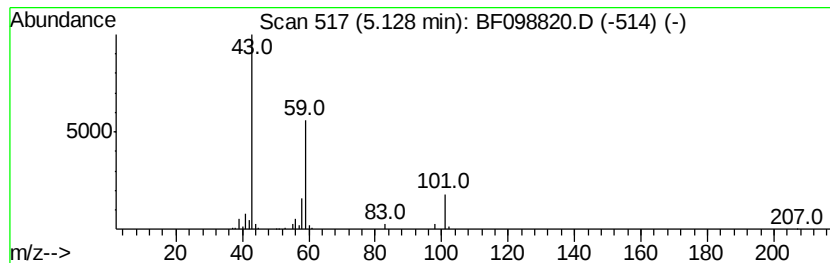
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	5.99 ng	239927	1,4-Dichlorobenzene-d4	6.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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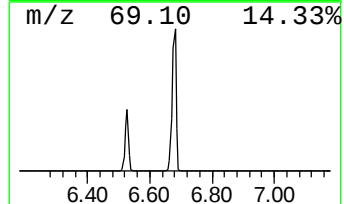
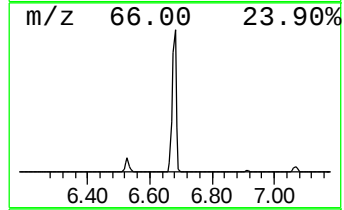
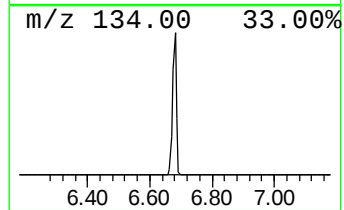
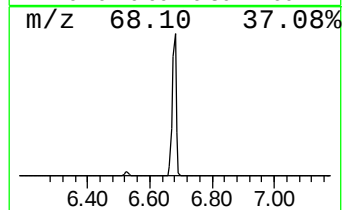
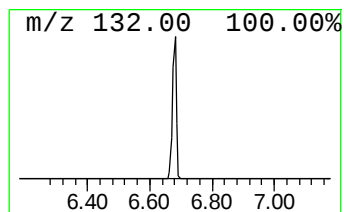
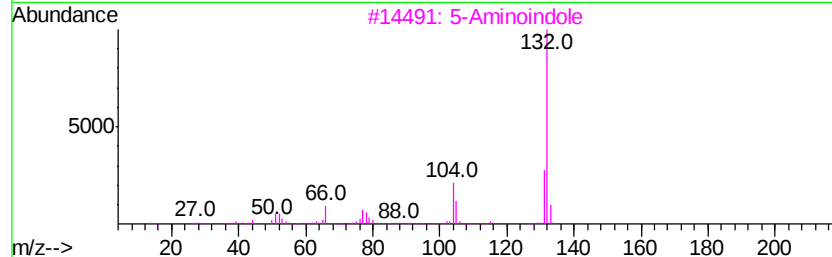
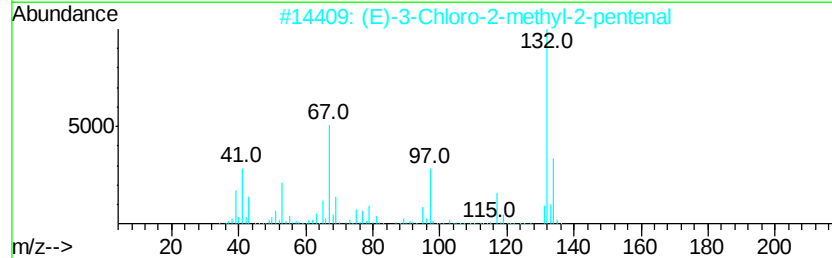
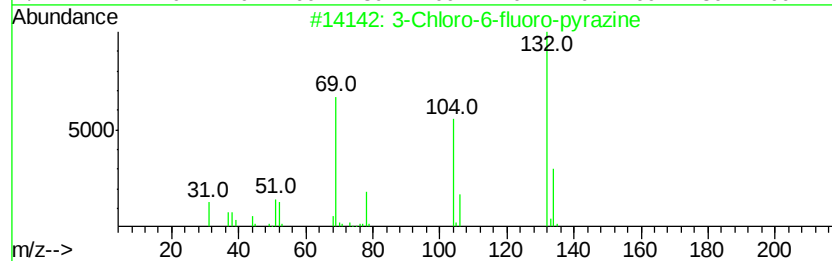
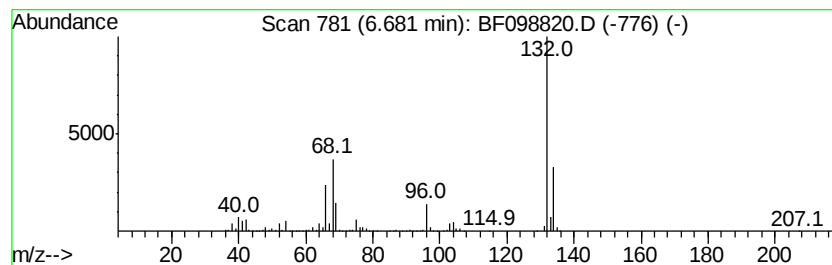
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Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	63.53 ng	2544570	1,4-Dichlorobenzene-d4	6.91

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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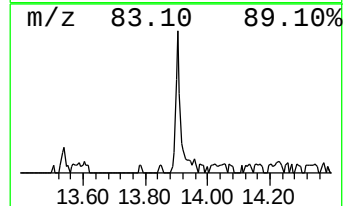
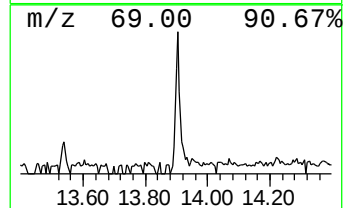
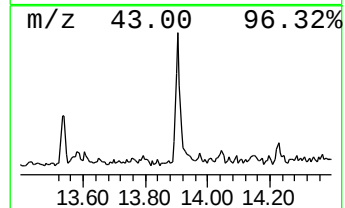
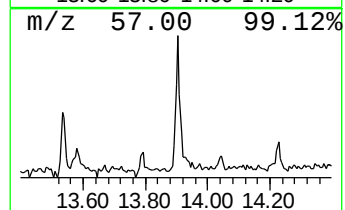
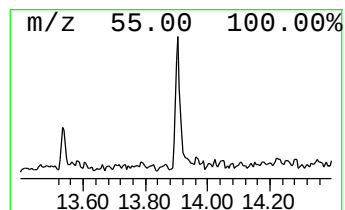
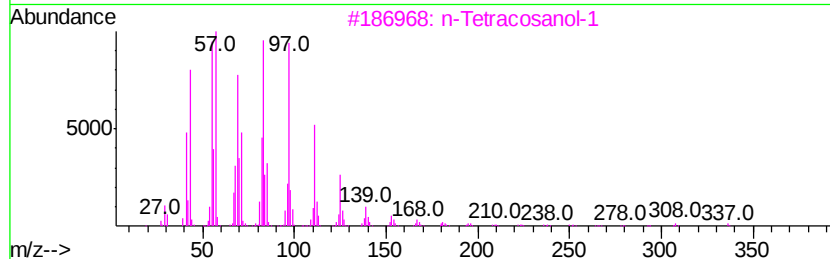
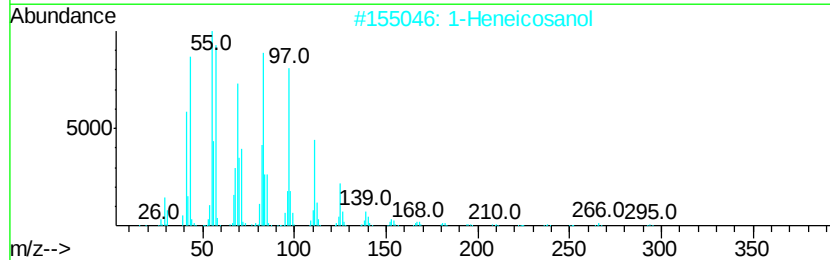
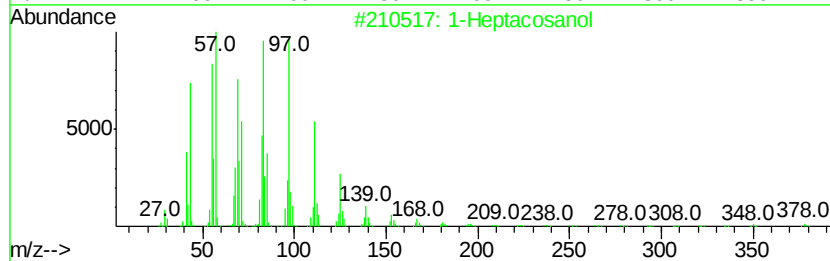
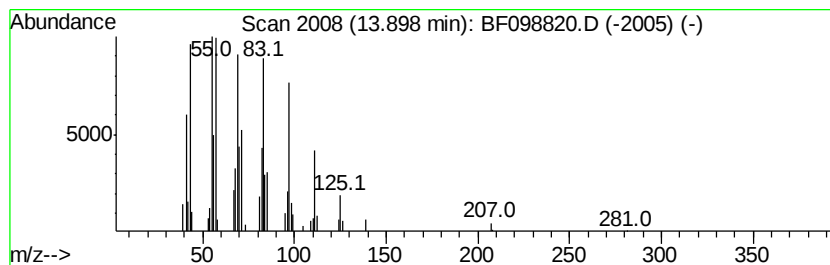
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Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.73 ng	90009	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.21	9.4	ng	377883	1	6.91	801040	20.0
2-Pentanone, 4-hy...	5.13	6.0	ng	239927	1	6.91	801040	20.0
unknown6.68	6.68	63.5	ng	2544570	1	6.91	801040	20.0
1-Heptacosanol	13.90	2.7	ng	90009	5	14.07	659657	20.0