

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
 Data File : BF098884.D
 Acq On : 28 Sep 2017 1:17
 Operator : SJ/JU
 Sample : I5419-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-TP-106V(0-5)

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-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	2.228	19	24	30	rVB	106316	141357	3.83%	0.440%
2	2.363	42	47	60	rVB3	22078	43964	1.19%	0.137%
3	5.151	516	521	533	rVB	563979	789492	21.40%	2.457%
4	5.540	582	587	590	rBV	3394775	3626948	98.32%	11.287%
5	6.545	752	758	761	rBV	3164518	3688980	100.00%	11.480%
6	6.687	777	782	785	rBV	3730264	3672927	99.56%	11.430%
7	6.916	817	821	824	rBV	1097366	863865	23.42%	2.688%
8	7.075	843	848	851	rBV	2808398	2646370	71.74%	8.235%
9	7.475	911	916	919	rBV	2182447	2324630	63.02%	7.234%
10	8.198	1035	1039	1042	rBV	1294868	1153608	31.27%	3.590%
11	9.269	1216	1221	1225	rBV	3556421	3463581	93.89%	10.778%
12	9.663	1283	1288	1291	rBV	546769	488546	13.24%	1.520%
13	9.951	1333	1337	1341	rBV	1331492	1191131	32.29%	3.707%
14	10.375	1406	1409	1412	rVB	53596	42095	1.14%	0.131%
15	10.739	1467	1471	1475	rBV	1939876	1906411	51.68%	5.932%
16	10.845	1486	1489	1494	rBV	74956	68212	1.85%	0.212%
17	11.439	1586	1590	1593	rBV	1300034	1056760	28.65%	3.288%
18	11.951	1673	1677	1682	rBV2	62612	63880	1.73%	0.199%
19	12.651	1793	1796	1800	rBV	74347	61346	1.66%	0.191%
20	12.880	1830	1835	1838	rBV	68742	65639	1.78%	0.204%
21	13.027	1855	1860	1863	rBV	2853757	2730606	74.02%	8.497%
22	13.904	2006	2009	2018	rBV	253307	257112	6.97%	0.800%
23	14.045	2030	2033	2035	rBV	50161	45706	1.24%	0.142%
24	14.080	2035	2039	2042	rVV	969091	870512	23.60%	2.709%
25	14.539	2114	2117	2120	rBV3	30969	37588	1.02%	0.117%
26	14.827	2163	2166	2173	rVB2	54269	64221	1.74%	0.200%
27	15.568	2287	2292	2303	rVB2	535254	722510	19.59%	2.248%
28	16.027	2367	2370	2375	rVB2	33014	47274	1.28%	0.147%

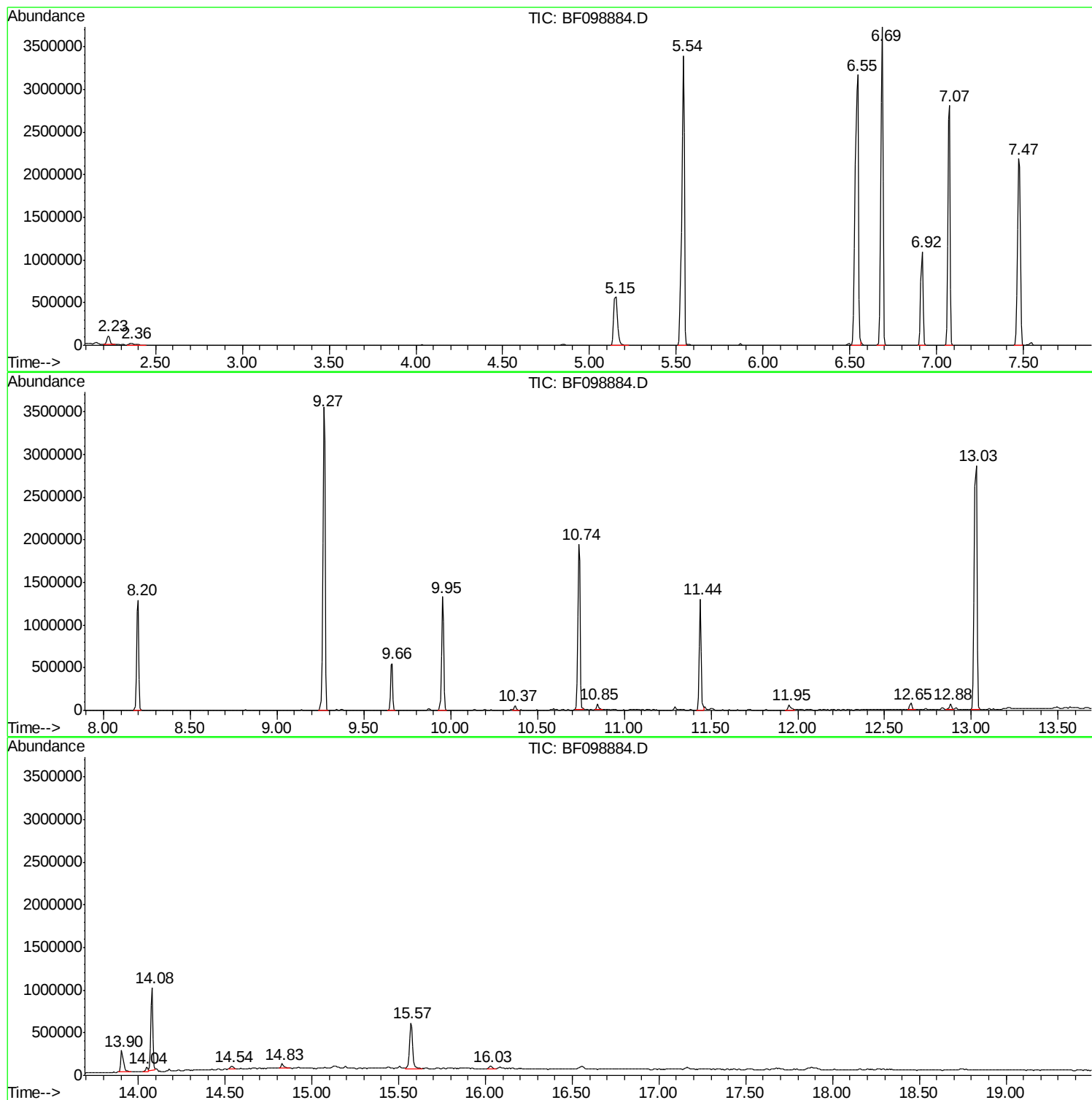
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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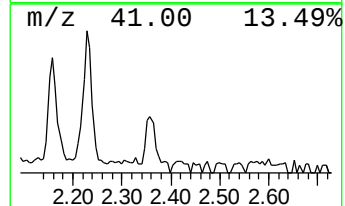
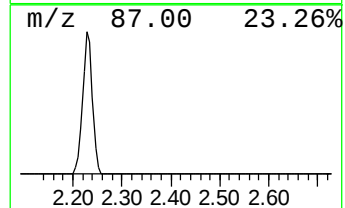
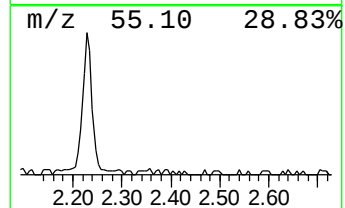
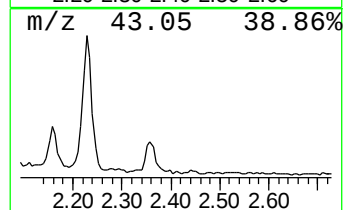
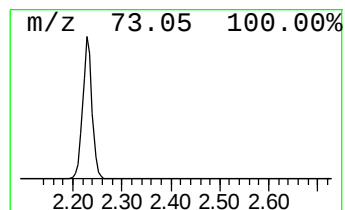
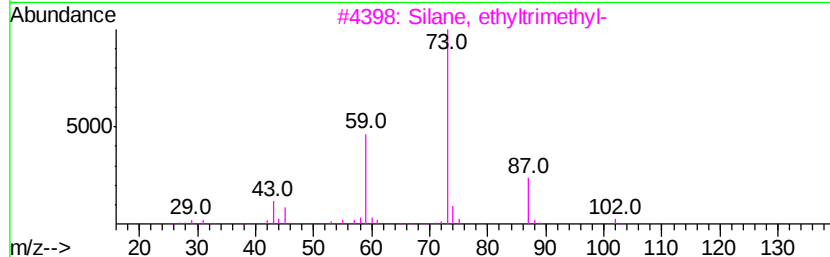
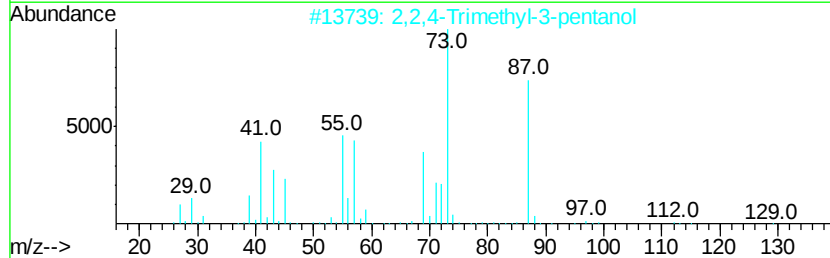
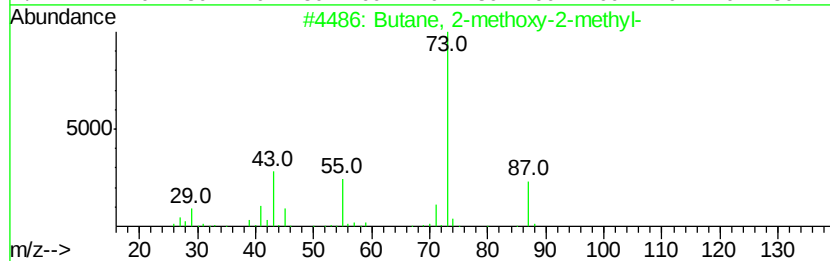
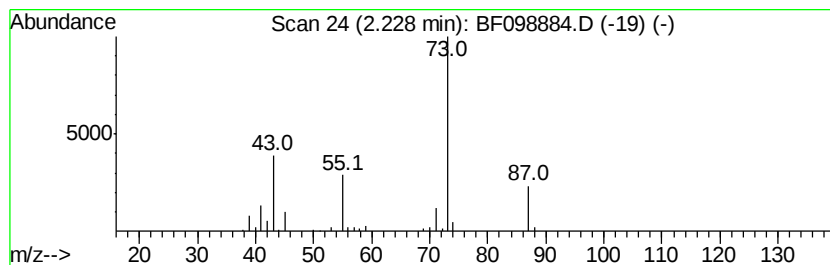
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	3.27 ng	141357	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25



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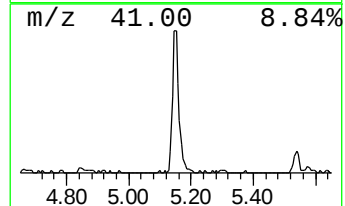
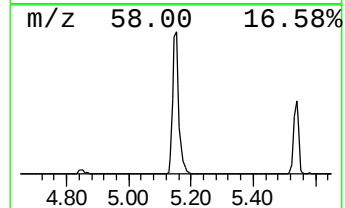
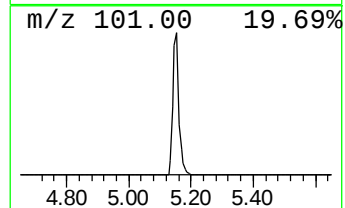
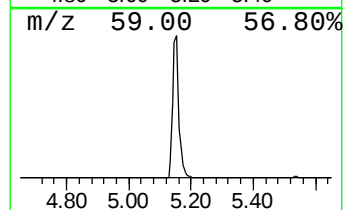
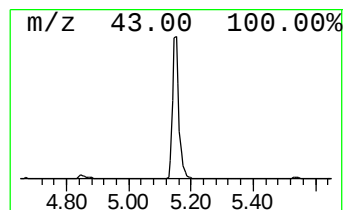
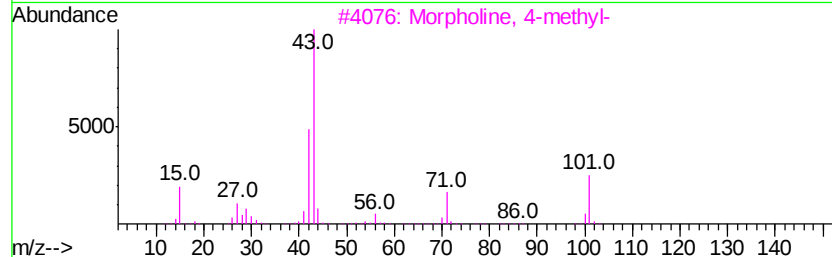
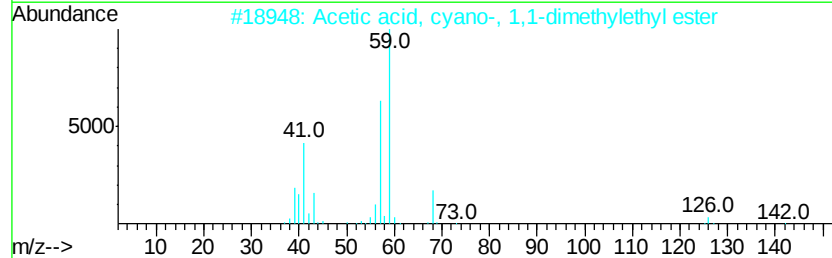
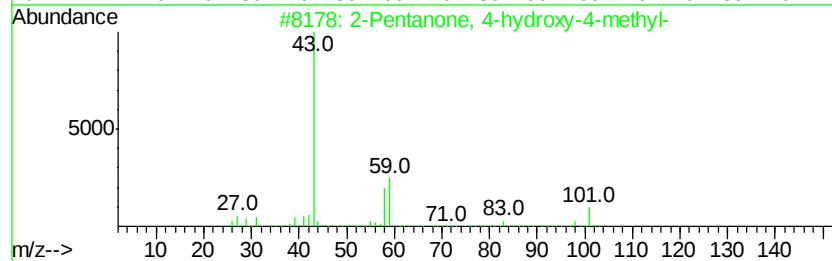
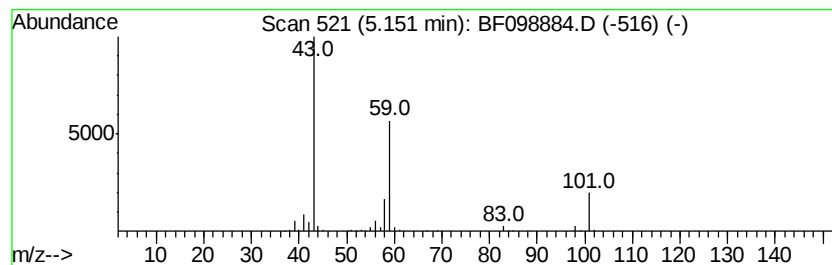
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	18.28 ng	789492	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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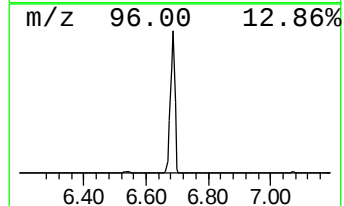
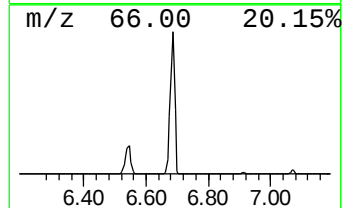
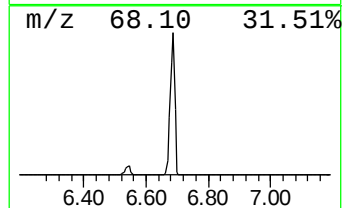
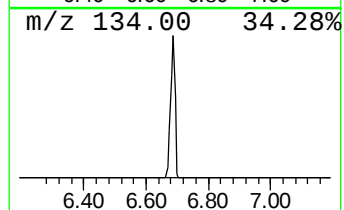
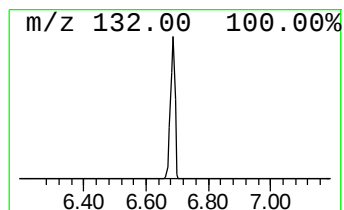
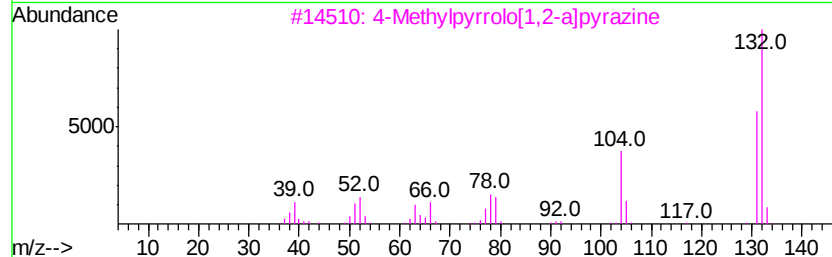
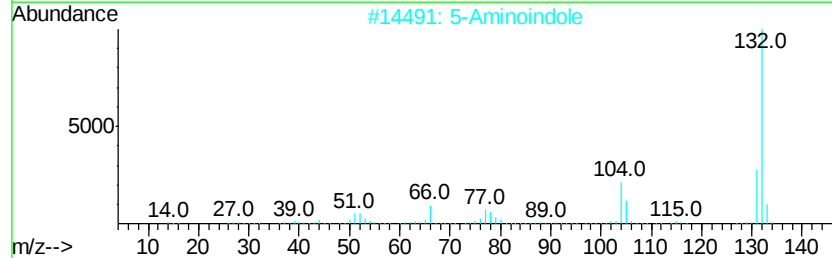
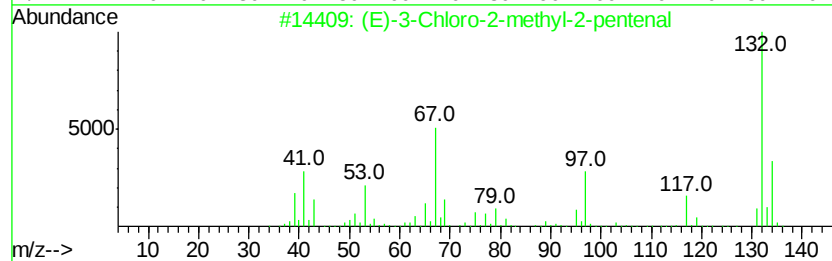
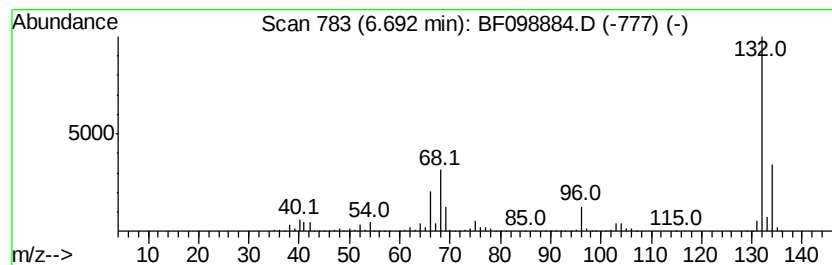
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Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	85.03 ng	3672930	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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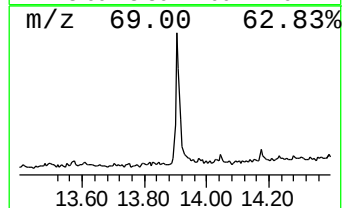
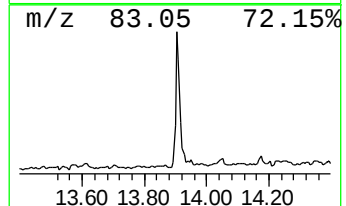
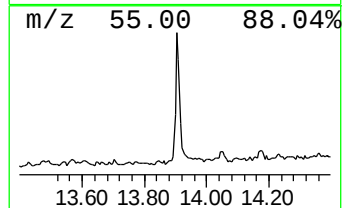
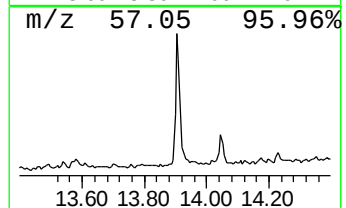
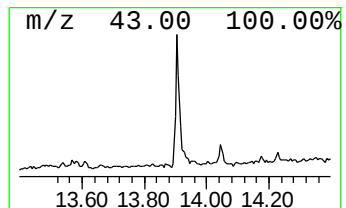
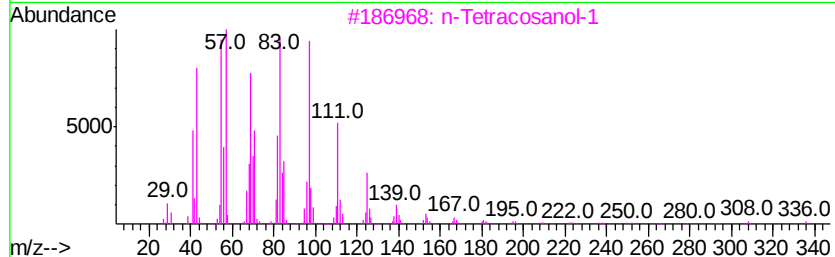
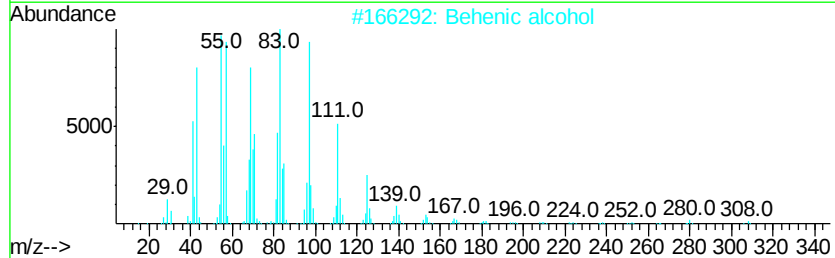
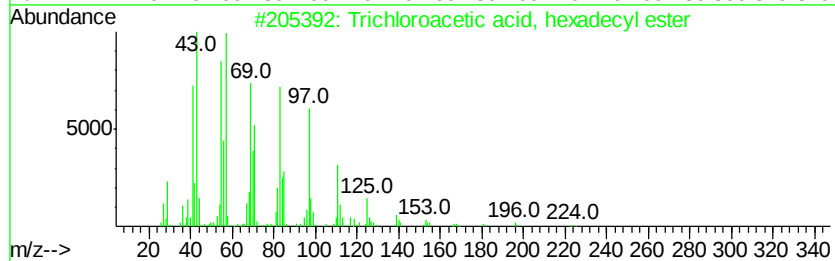
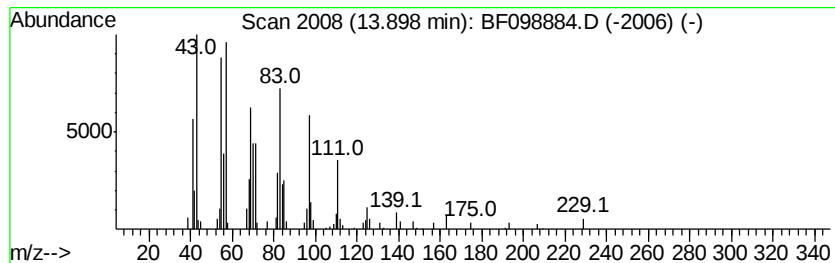
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Peak Number 5 Trichloroacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	5.91 ng	257112	Chrysene-d12	14.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.23	3.3	ng	141357	1	6.92	863865	20.0
2-Pentanone, 4-hy...	5.15	18.3	ng	789492	1	6.92	863865	20.0
unknown6.69	6.69	85.0	ng	3672930	1	6.92	863865	20.0
Trichloroacetic a...	13.90	5.9	ng	257112	5	14.08	870512	20.0