

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
 Data File : BF098793.D
 Acq On : 25 Sep 2017 20:07
 Operator : SJ/JU
 Sample : I5395-16
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6-(0-5)

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	2.246	23	27	44	rVB2	124596	246032	7.05%	0.765%
2	5.145	516	520	531	rVB	475099	603308	17.29%	1.875%
3	5.534	581	586	589	rBV	3002335	3245461	93.03%	10.086%
4	6.534	750	756	761	rBV	2863474	3352865	96.11%	10.419%
5	6.681	776	781	784	rBV	3332502	3303312	94.69%	10.266%
6	6.910	817	820	824	rBV	925046	790827	22.67%	2.458%
7	7.069	843	847	850	rBV	2761508	2390805	68.53%	7.430%
8	7.475	910	916	919	rBV	2094406	2018322	57.86%	6.272%
9	8.192	1034	1038	1042	rBV	1213461	1060824	30.41%	3.297%
10	9.269	1215	1221	1224	rBV	3572462	3356015	96.20%	10.429%
11	9.657	1283	1287	1290	rBV	541316	429219	12.30%	1.334%
12	9.951	1332	1337	1341	rVB	1298974	1151405	33.01%	3.578%
13	10.374	1401	1409	1412	rBV2	54207	58022	1.66%	0.180%
14	10.739	1464	1471	1474	rBV	2204448	2130671	61.08%	6.621%
15	10.845	1486	1489	1494	rBV	69926	63844	1.83%	0.198%
16	11.439	1585	1590	1593	rBV	1358902	1190256	34.12%	3.699%
17	11.951	1673	1677	1681	rBV	76639	67585	1.94%	0.210%
18	13.021	1854	1859	1863	rBV	3386811	3488567	100.00%	10.841%
19	13.904	2005	2009	2017	rBV	398154	373328	10.70%	1.160%
20	14.074	2034	2038	2041	rBV	1419220	1218072	34.92%	3.785%
21	14.539	2113	2117	2122	rBV3	33910	48143	1.38%	0.150%
22	14.921	2179	2182	2187	rBV	51506	52290	1.50%	0.162%
23	15.192	2224	2228	2231	rBV	30670	36301	1.04%	0.113%
24	15.568	2286	2292	2303	rVB	901181	1162157	33.31%	3.612%
25	16.027	2366	2370	2375	rBV	44072	65848	1.89%	0.205%
26	16.080	2375	2379	2387	rBV3	53102	85770	2.46%	0.267%
27	16.545	2454	2458	2465	rVB	41392	73484	2.11%	0.228%
28	17.162	2558	2563	2572	rVB4	30632	69481	1.99%	0.216%
29	17.886	2682	2686	2695	rVB4	22371	46544	1.33%	0.145%

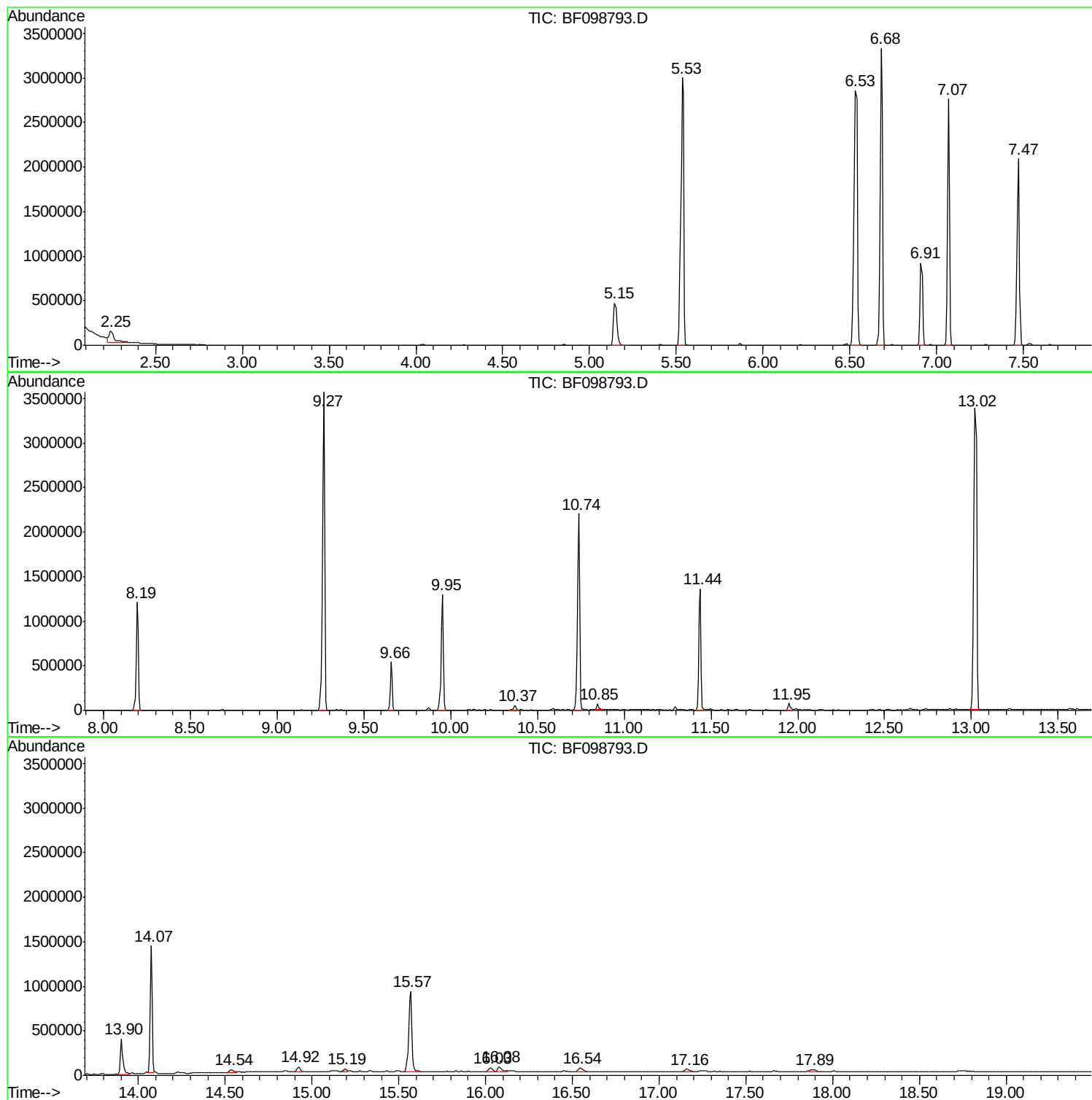
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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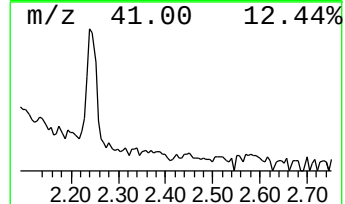
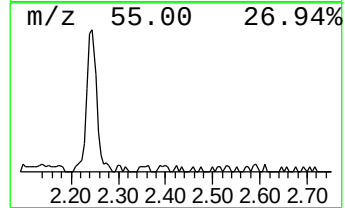
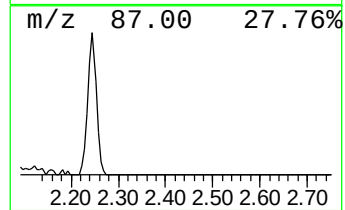
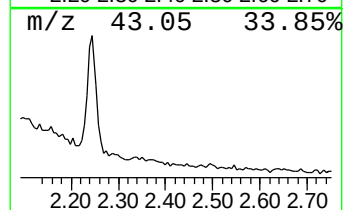
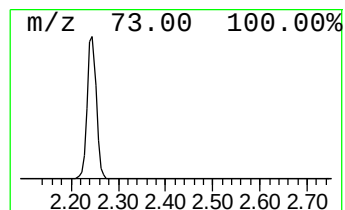
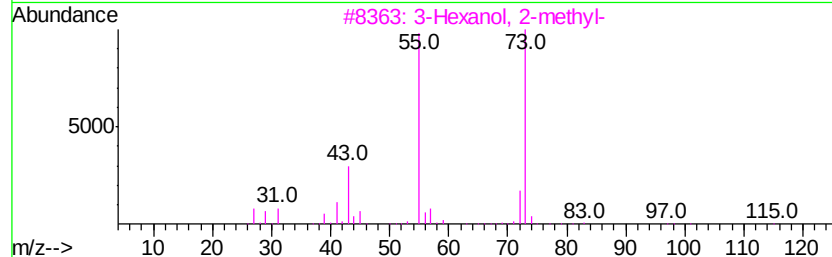
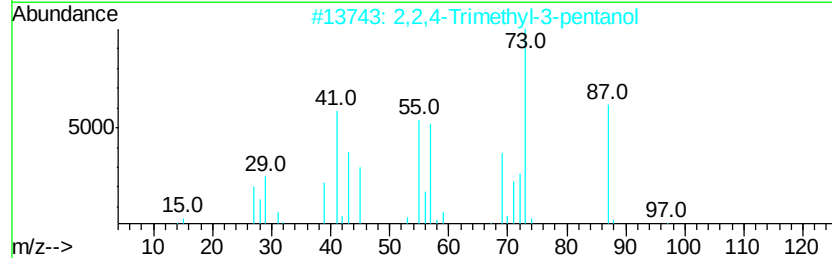
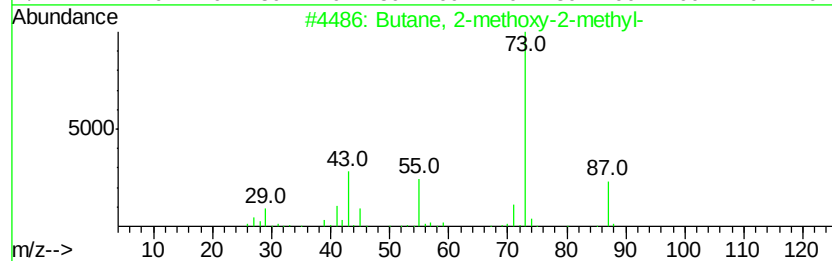
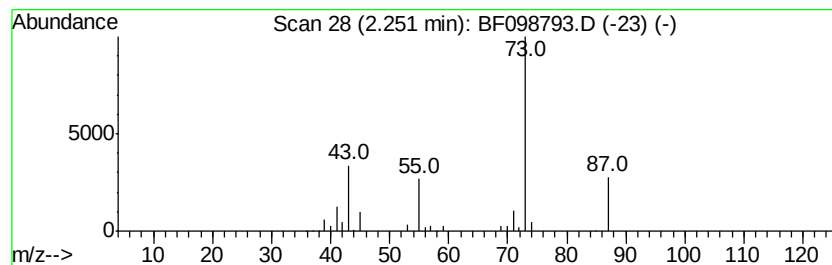
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	6.22 ng	246032	1,4-Dichlorobenzene-d4	6.91

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		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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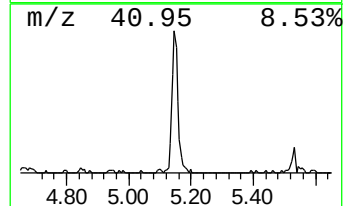
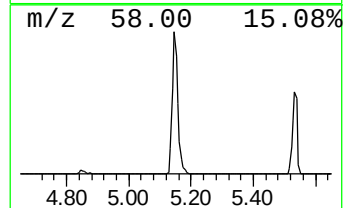
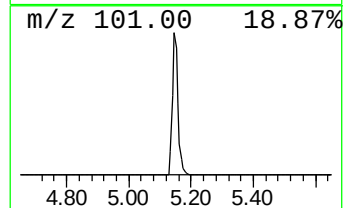
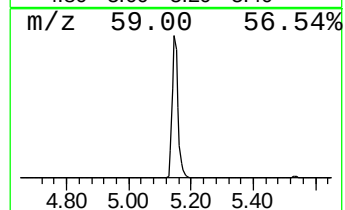
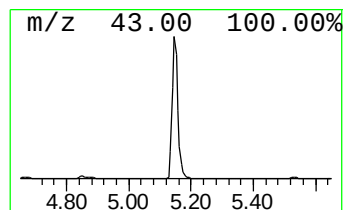
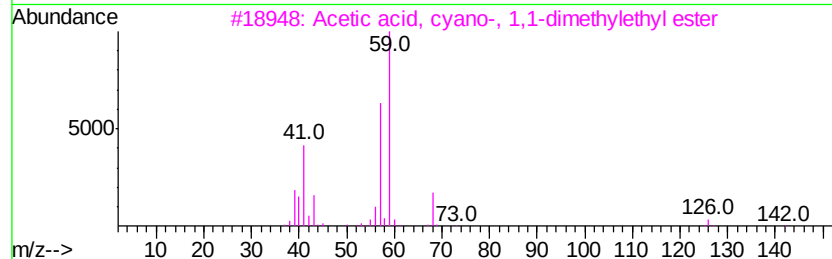
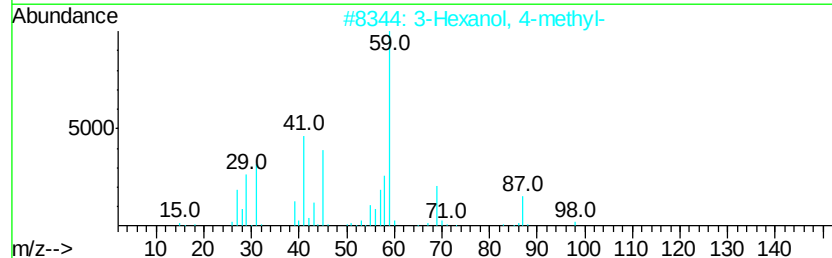
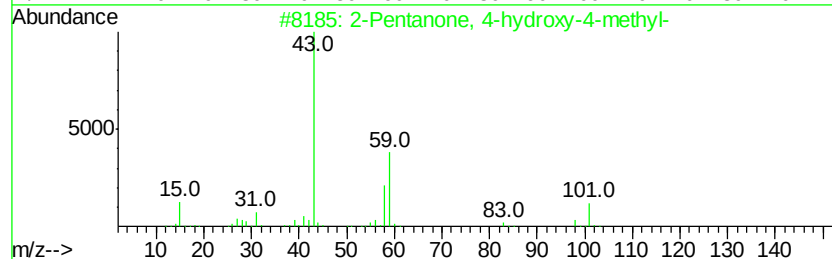
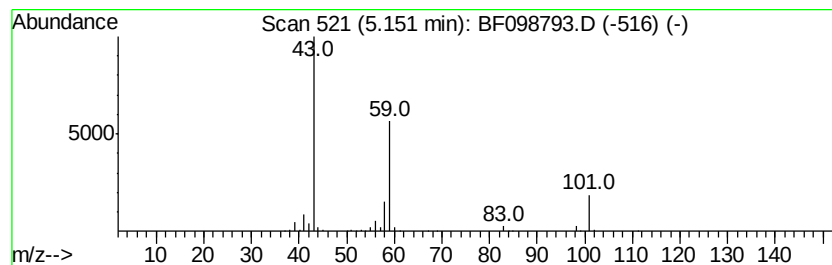
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.26 ng	603308	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	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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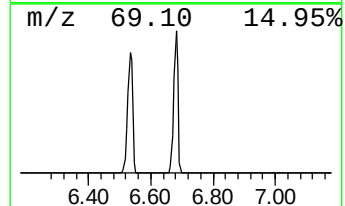
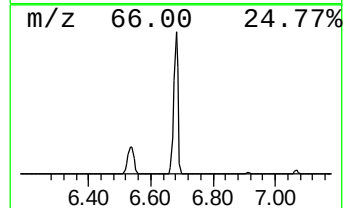
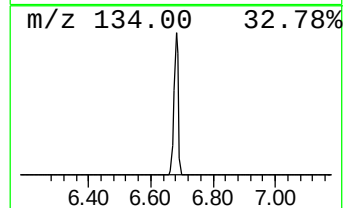
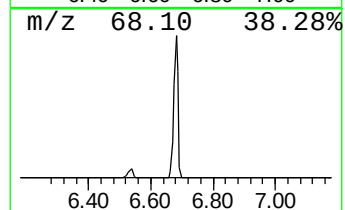
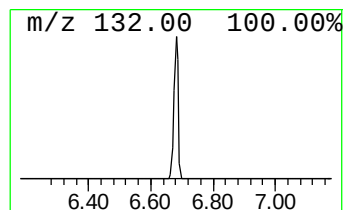
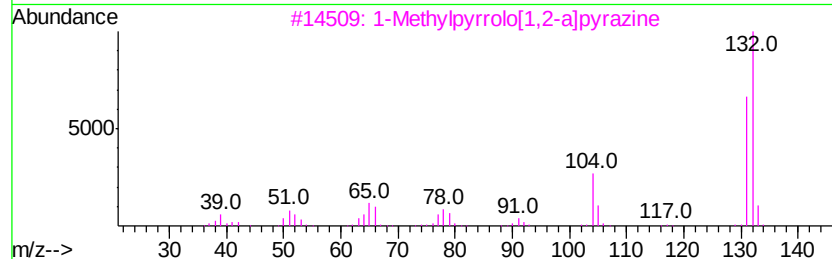
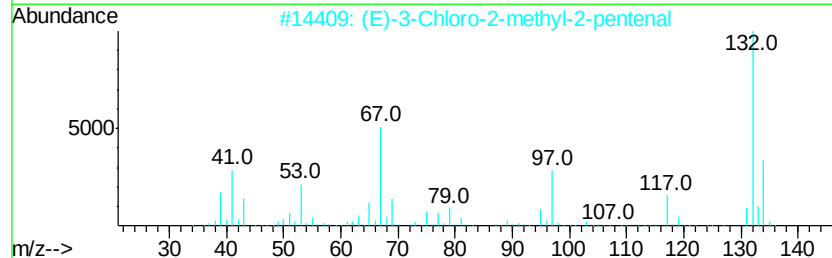
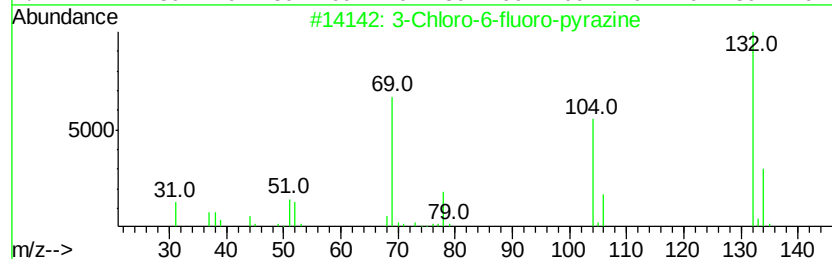
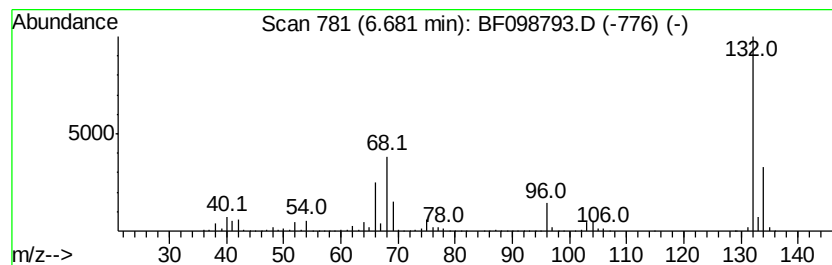
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Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	83.54 ng	3303310	1,4-Dichlorobenzene-d4	6.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	17
3	1-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9
4	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
5	Imidazole, 4,5-dicyano-1-methyl-			132	C6H4N4	019485-35-9	9



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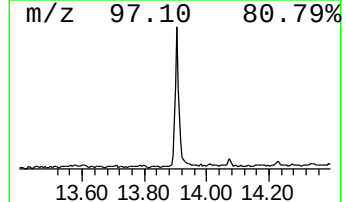
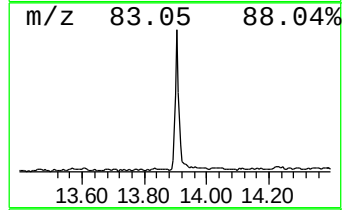
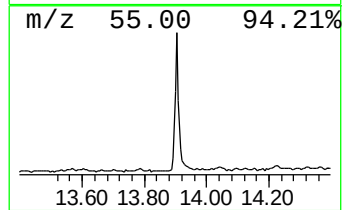
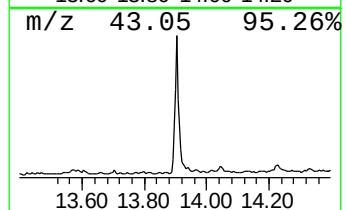
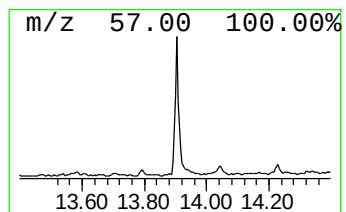
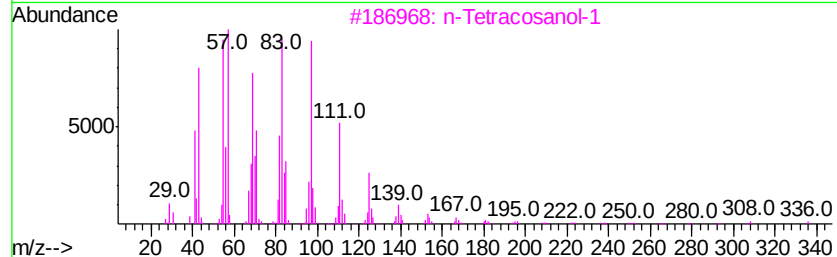
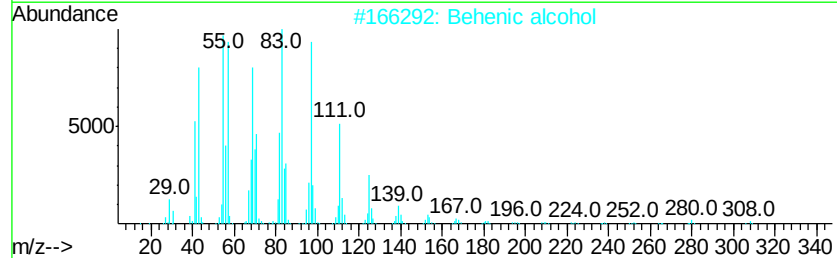
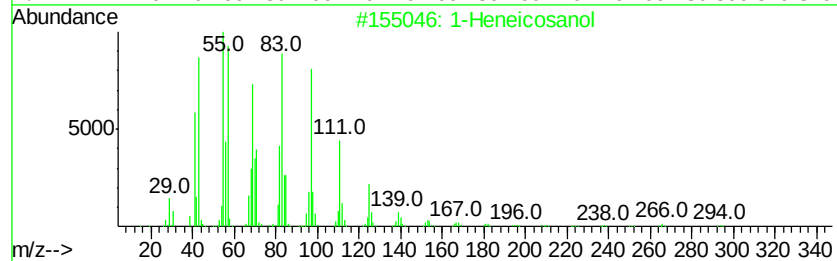
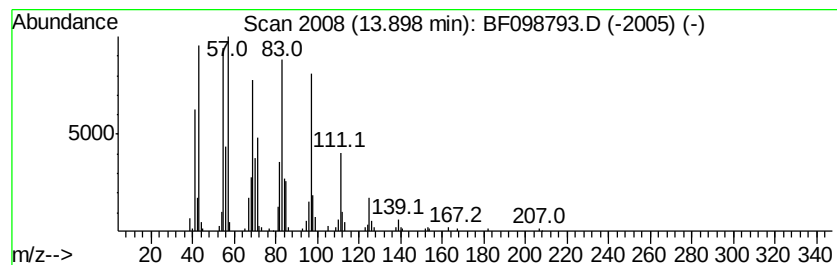
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	6.13 ng	373328	Chrysene-d12	14.07	
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	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.25	6.2	ng	246032	1	6.91	790827	20.0
2-Pentanone, 4-hy...	5.15	15.3	ng	603308	1	6.91	790827	20.0
unknown6.68	6.68	83.5	ng	3303310	1	6.91	790827	20.0
1-Heneicosanol	13.90	6.1	ng	373328	5	14.07	1218070	20.0