

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071421\
 Data File : BP006228.D
 Acq On : 14 Jul 2021 20:43
 Operator : CG/JU
 Sample : M3026-08
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 ABN-JG-3

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:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006228.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	208	213	243	rVB	1991835	2982838	17.85%	6.031%
2	4.975	312	321	338	rBV	9303684	16707603	100.00%	33.780%
3	7.058	670	675	696	rBV2	156696	413633	2.48%	0.836%
4	7.846	800	809	828	rBV	729069	1277980	7.65%	2.584%
5	9.022	1002	1009	1031	rBV	967407	1942986	11.63%	3.928%
6	10.469	1248	1255	1268	rBV	69167	217202	1.30%	0.439%
7	10.652	1278	1286	1303	rBV	998373	1816541	10.87%	3.673%
8	13.110	1695	1704	1722	rBV	2627121	4040900	24.19%	8.170%
9	14.487	1931	1938	1960	rVB	1385916	2242117	13.42%	4.533%
10	17.240	2399	2406	2411	rBV	1535626	2530126	15.14%	5.116%
11	17.281	2411	2413	2421	rVB	195374	288489	1.73%	0.583%
12	19.245	2742	2747	2754	rBV	384426	528102	3.16%	1.068%
13	19.598	2803	2807	2815	rVB	378655	500616	3.00%	1.012%
14	19.786	2833	2839	2848	rBV	5137516	6084802	36.42%	12.303%
15	21.016	3044	3048	3057	rBV5	197831	352383	2.11%	0.712%
16	21.316	3093	3099	3103	rBV	2564851	3424060	20.49%	6.923%
17	23.692	3496	3503	3521	rVB2	1948862	4109121	24.59%	8.308%

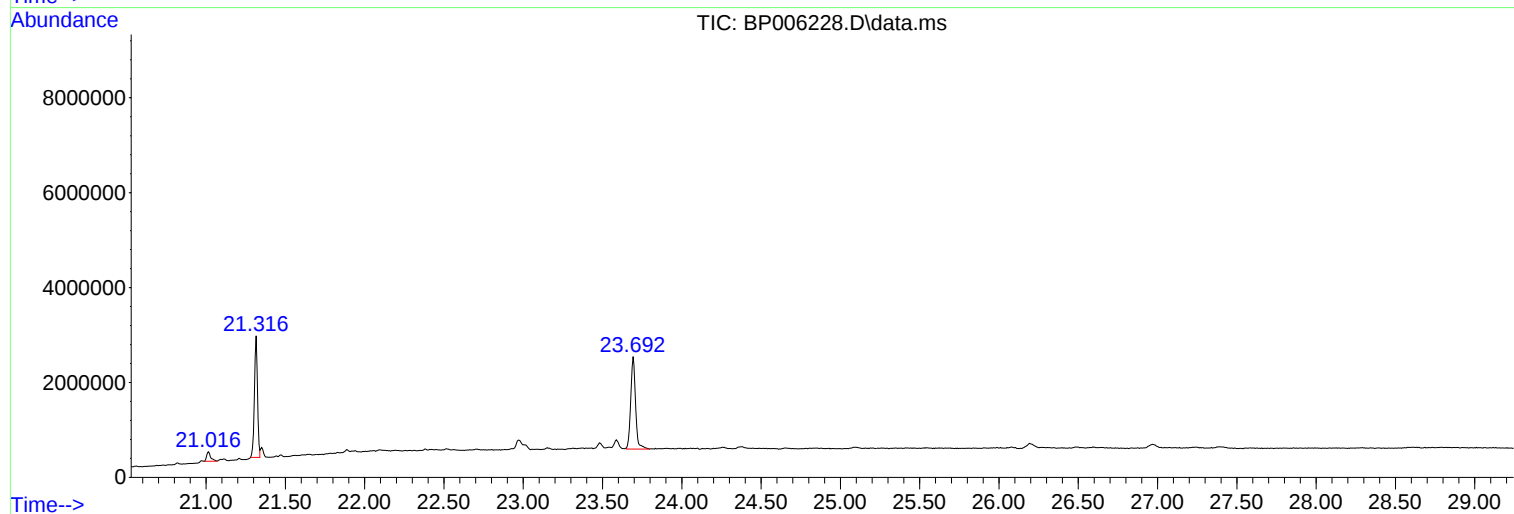
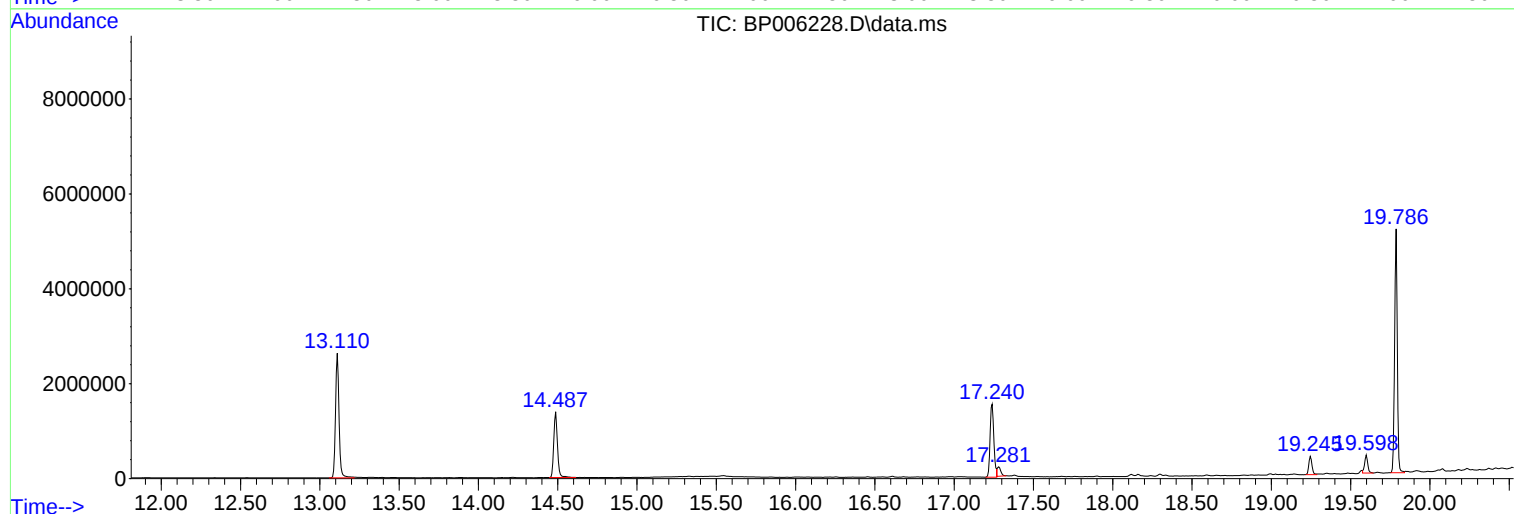
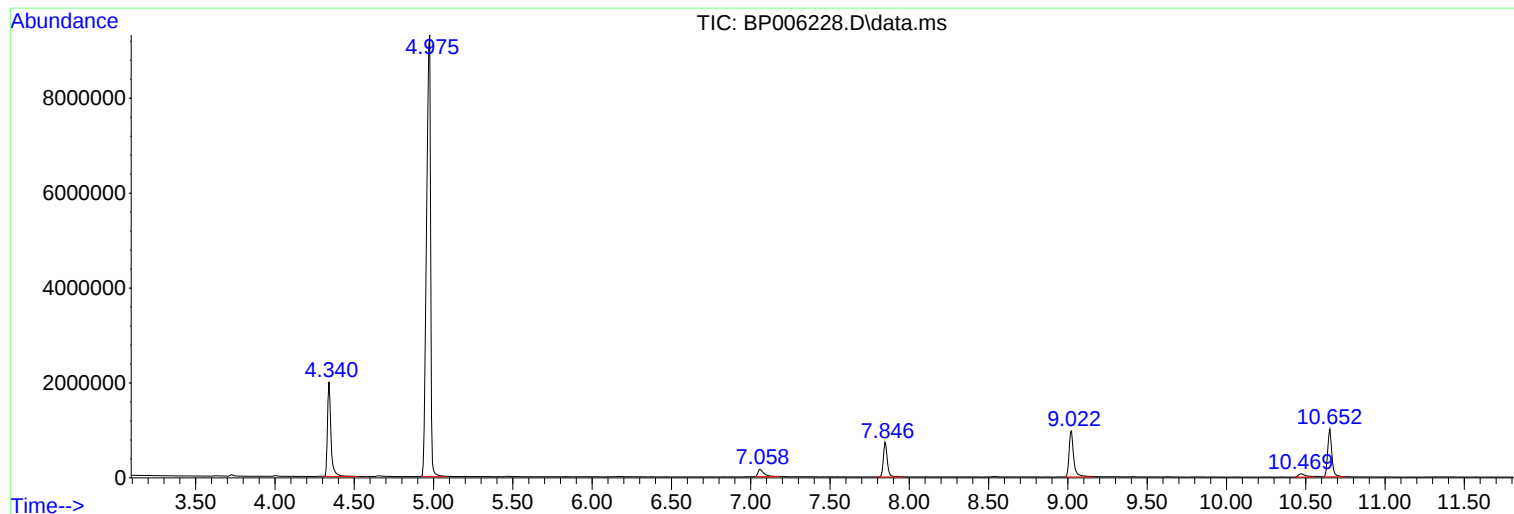
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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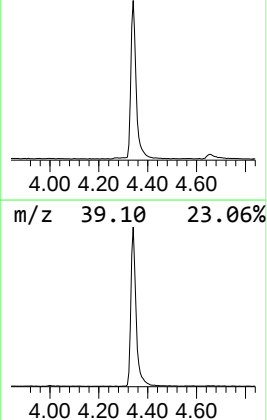
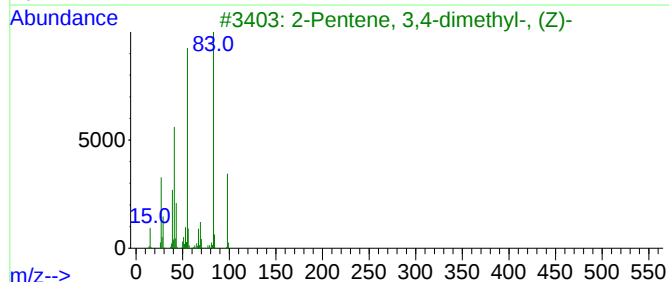
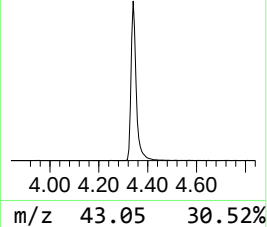
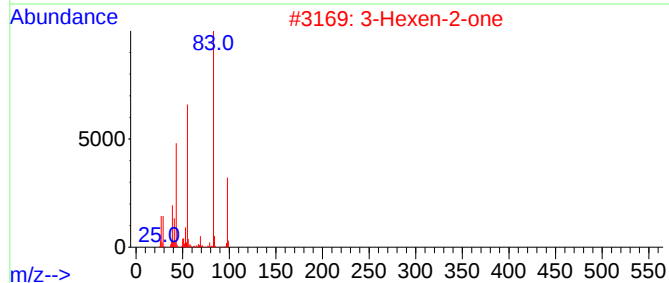
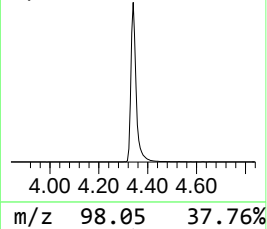
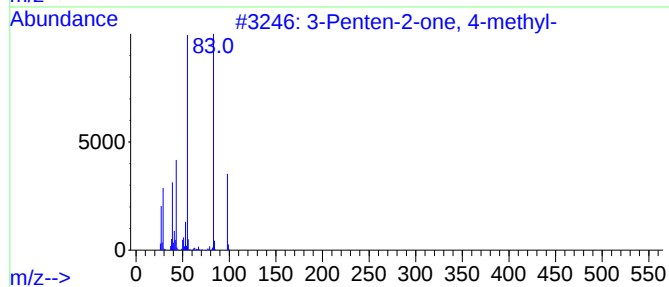
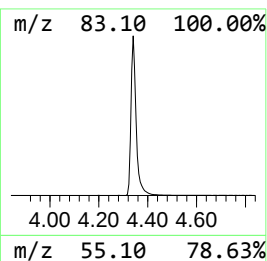
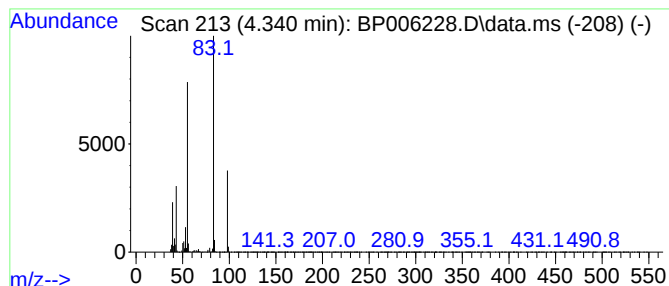
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	46.68 ng	2982840	1,4-Dichlorobenzene-d4	7.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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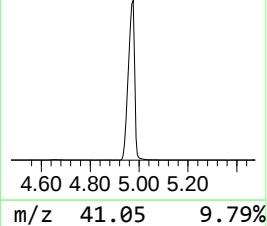
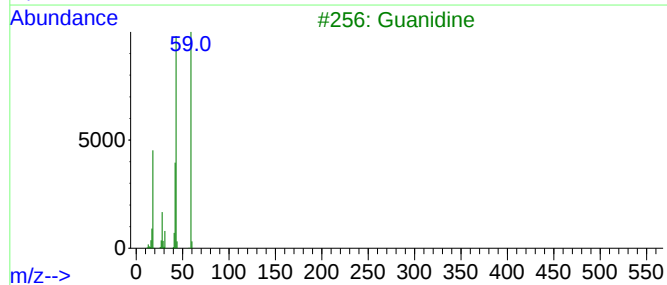
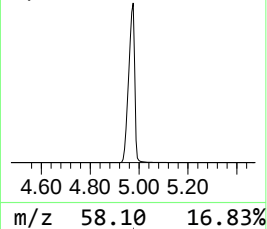
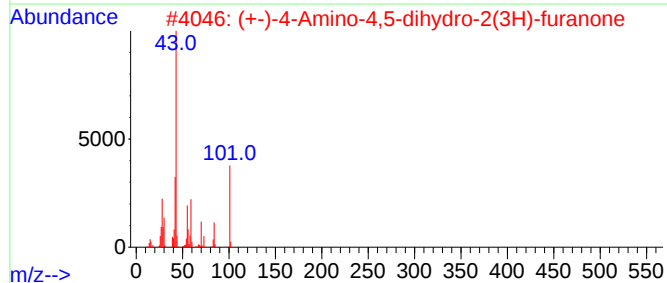
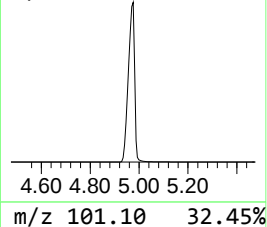
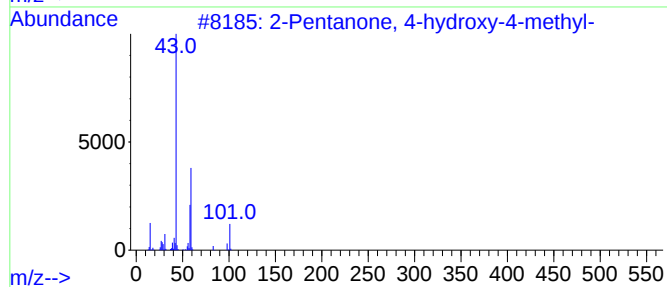
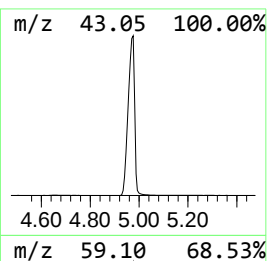
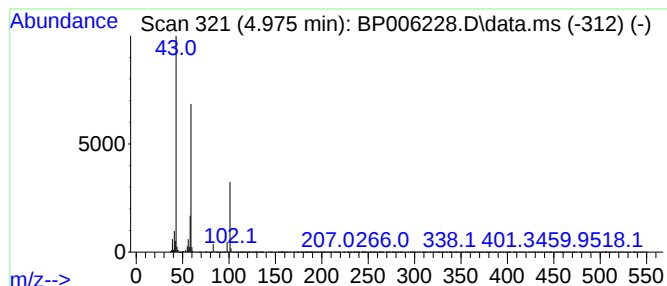
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	261.47 ng	16707600	1,4-Dichlorobenzene-d4	7.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1,2-Butanediol	90	C4H10O2	000584-03-2	23



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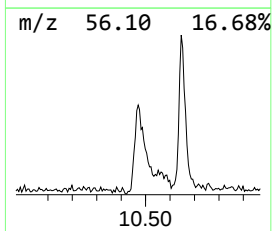
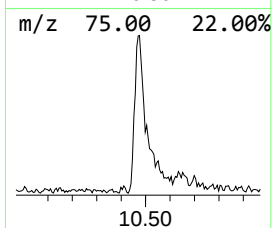
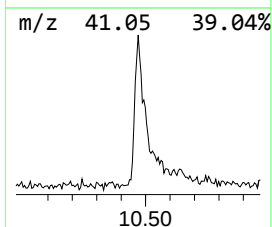
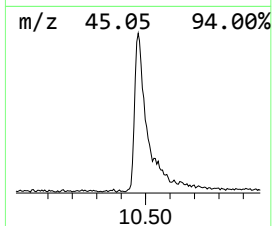
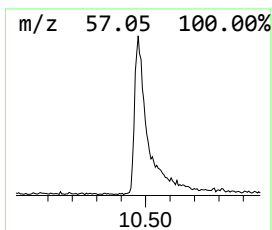
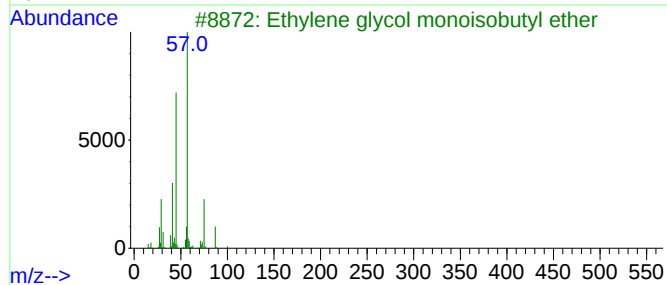
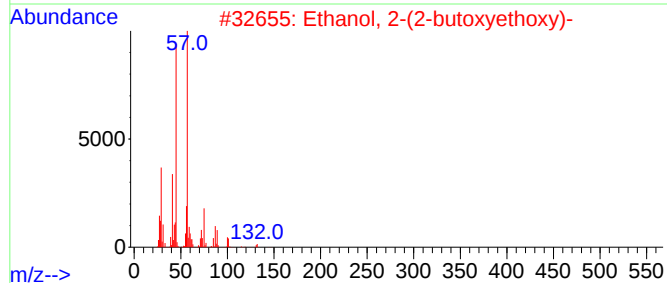
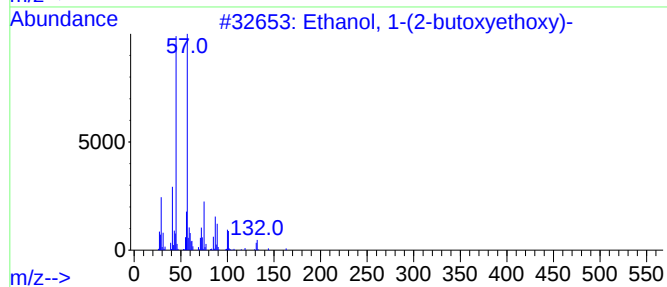
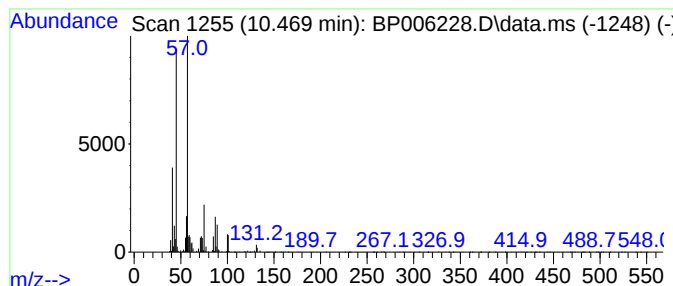
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Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	2.39 ng	217202	Naphthalene-d8	10.652

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Methyl-2,3,5-tri-O-methyl-4-thio...	222	C9H18O4S	051306-30-0	53
5			Di-sec-butyl ether	130	C8H18O	006863-58-7	50



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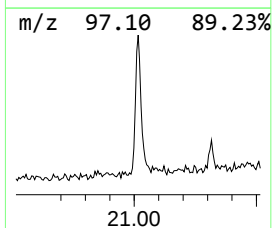
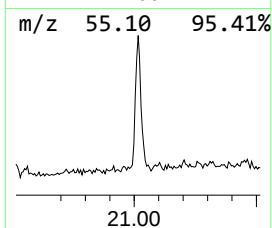
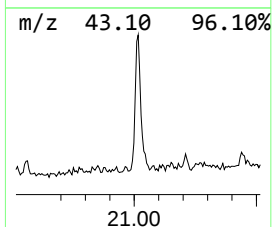
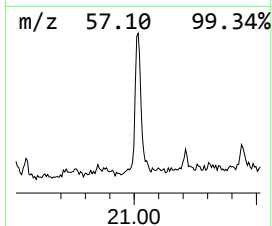
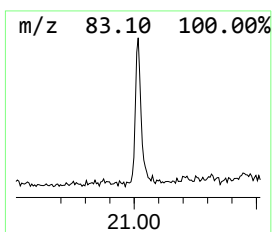
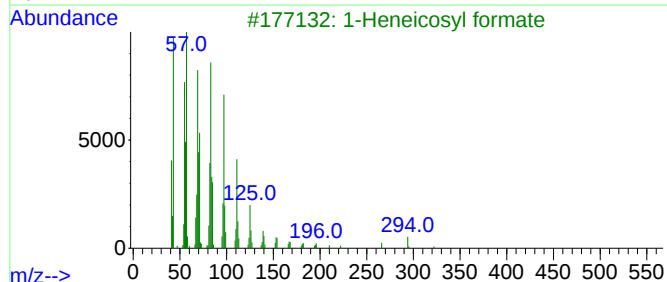
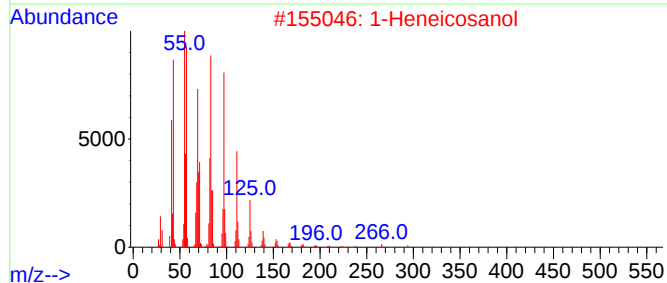
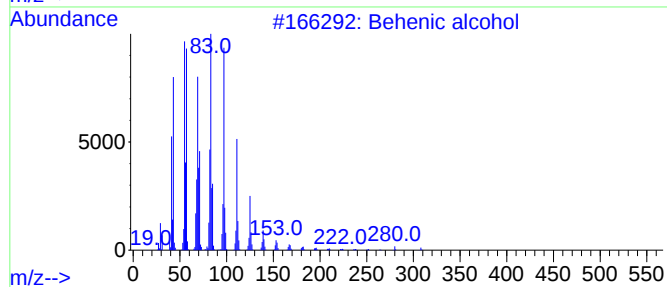
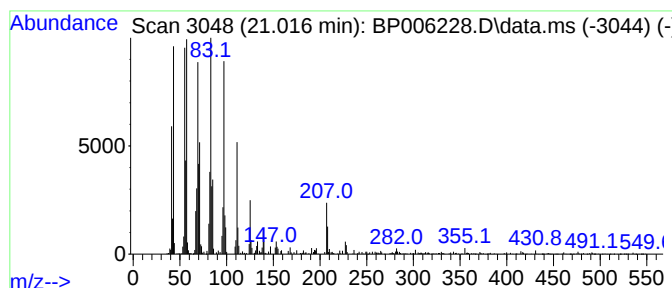
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Peak Number 4 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.016	2.06 ng	352383	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
4			1-Heptacosanol	396	C27H56O	002004-39-9	93
5			9-Tricosene, (Z)-	322	C23H46	027519-02-4	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.340	46.7	ng	2982840	1	7.846	1277980	20.0
2-Pentanone, 4-...	4.975	261.5	ng	16707600	1	7.846	1277980	20.0
Ethanol, 1-(2-b...	10.469	2.4	ng	217202	2	10.652	1816540	20.0
Behenic alcohol	21.016	2.1	ng	352383	5	21.316	3424060	20.0