

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
 Data File : BG055843.D
 Acq On : 30 Nov 2022 15:43
 Operator : CG/JU
 Sample : N5806-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-2

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_G\Methods\8270-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.648	225	231	238	rBV	15955	24879	1.36%	0.228%
2	5.270	329	337	350	rBV	408869	632901	34.64%	5.788%
3	5.752	412	419	428	rBV	481507	775222	42.43%	7.089%
4	6.369	517	524	533	rBV	25907	40552	2.22%	0.371%
5	7.368	687	694	712	rBV	484141	852374	46.65%	7.795%
6	8.220	832	839	847	rVB	122318	202357	11.08%	1.850%
7	9.389	1030	1038	1052	rBV	290512	520014	28.46%	4.755%
8	11.046	1313	1320	1328	rBV	171314	308554	16.89%	2.822%
9	13.467	1725	1732	1741	rBV	800070	1206567	66.04%	11.034%
10	14.841	1959	1966	1974	rVB	308753	477709	26.15%	4.368%
11	16.181	2189	2194	2200	rVB2	12659	21565	1.18%	0.197%
12	16.328	2212	2219	2231	rBV	678040	1070370	58.58%	9.788%
13	16.534	2247	2254	2259	rVB	16524	26925	1.47%	0.246%
14	17.168	2358	2362	2367	rVB2	15378	23675	1.30%	0.216%
15	17.585	2426	2433	2437	rBV	385190	607925	33.27%	5.559%
16	17.626	2437	2440	2445	rVB	54992	76165	4.17%	0.697%
17	18.443	2573	2579	2586	rBV3	60621	117511	6.43%	1.075%
18	18.502	2586	2589	2595	rVB3	17635	30902	1.69%	0.283%
19	18.649	2609	2614	2618	rBV3	15990	29203	1.60%	0.267%
20	19.354	2730	2734	2739	rBV2	16708	29193	1.60%	0.267%
21	19.624	2774	2780	2784	rBV	123652	182446	9.99%	1.668%
22	19.700	2790	2793	2799	rBV7	17422	28856	1.58%	0.264%
23	19.983	2837	2841	2849	rVB	127965	187107	10.24%	1.711%
24	20.171	2867	2873	2878	rBV	1374747	1827068	100.00%	16.708%
25	20.447	2917	2920	2922	rBV2	19903	25106	1.37%	0.230%
26	20.946	3002	3005	3008	rVB	24485	28672	1.57%	0.262%
27	21.469	3091	3094	3098	rBV3	40093	53301	2.92%	0.487%
28	21.869	3155	3162	3168	rBV2	391420	761370	41.67%	6.962%
29	21.921	3168	3171	3177	rVB	54504	83297	4.56%	0.762%
30	22.156	3208	3211	3215	rVB2	30523	38853	2.13%	0.355%
31	25.259	3730	3739	3750	rVB2	215817	644752	35.29%	5.896%

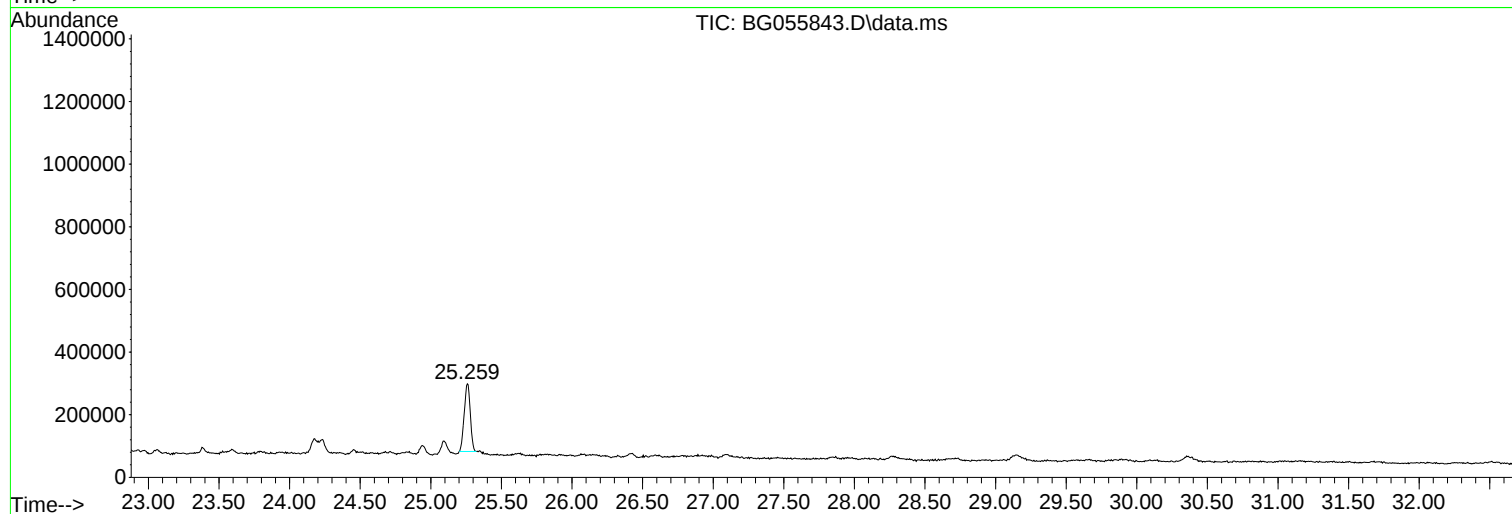
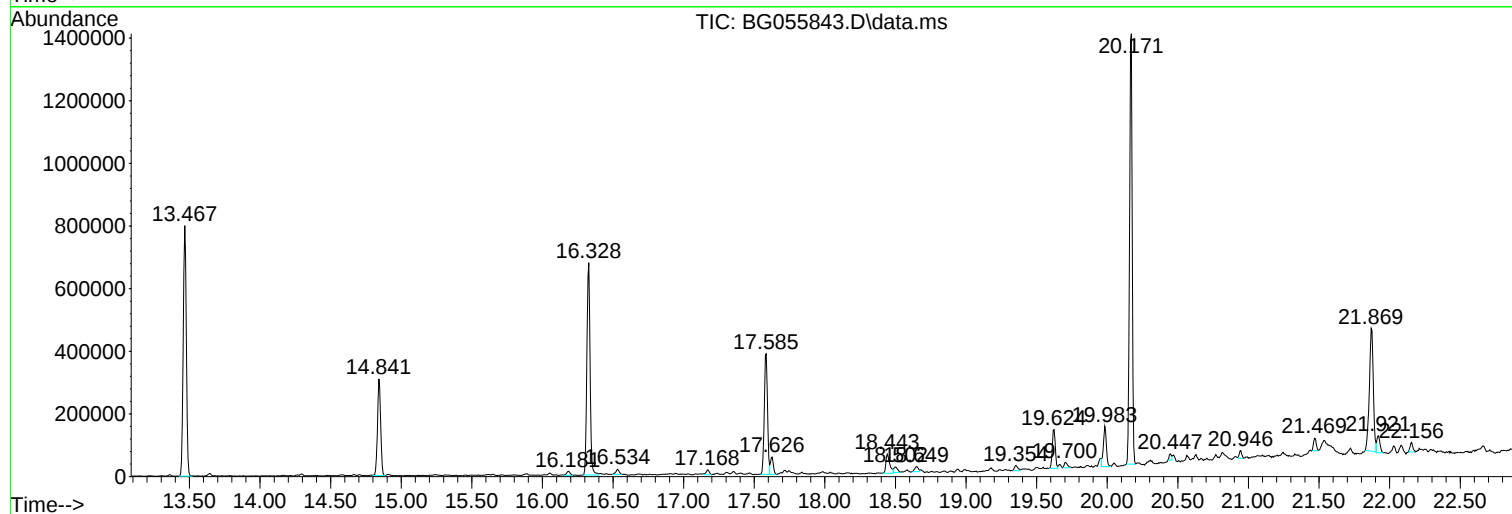
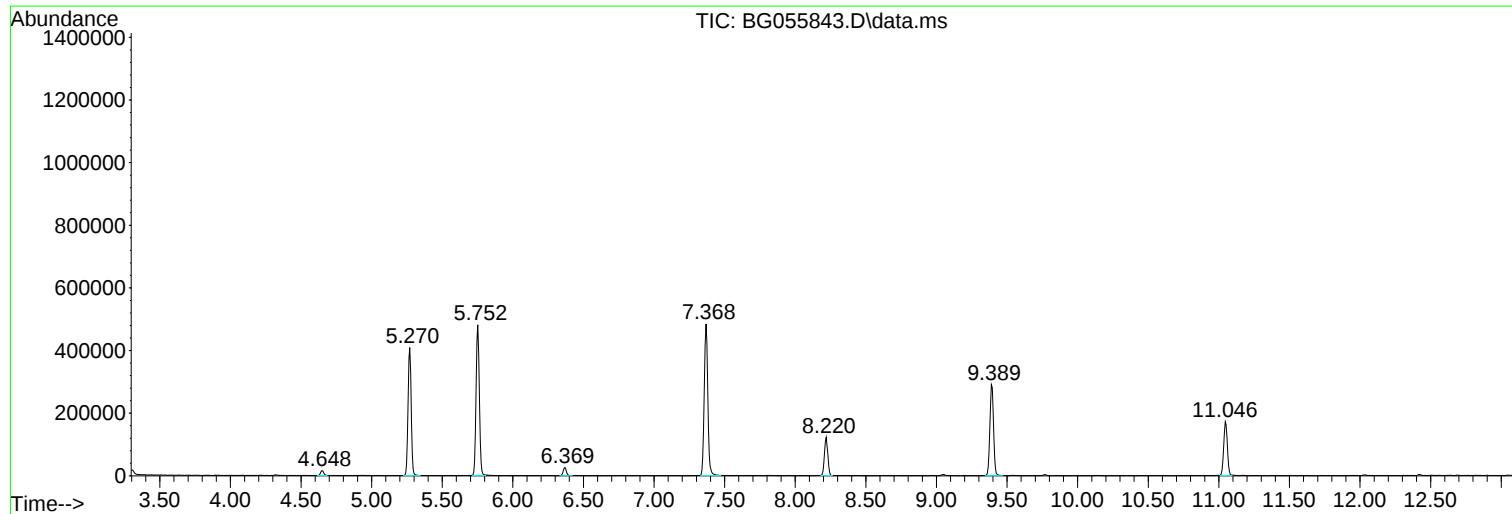
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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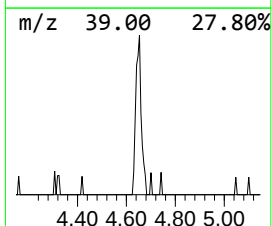
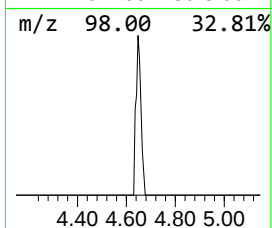
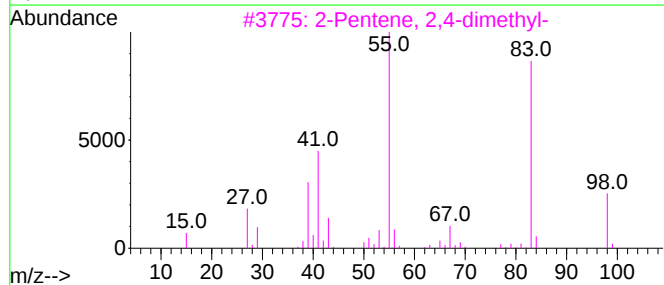
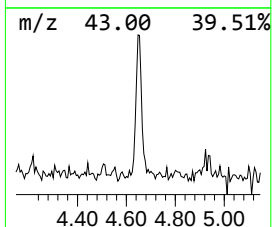
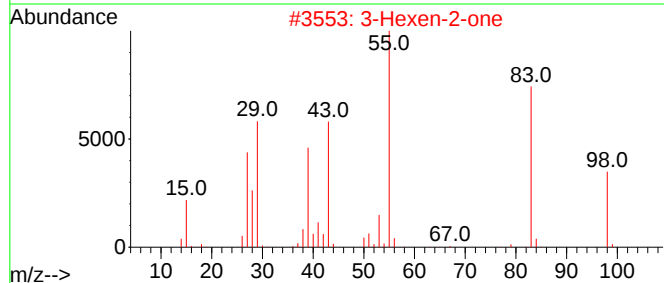
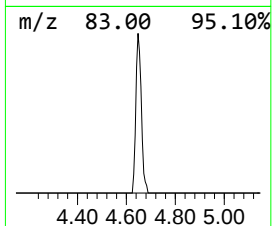
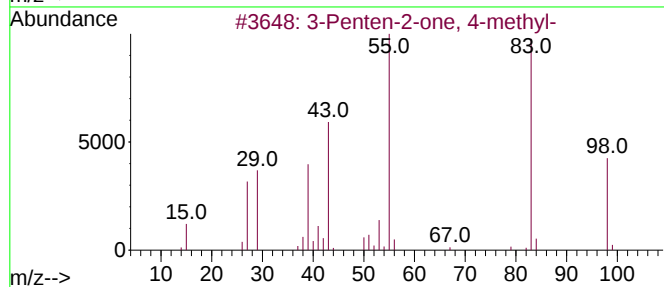
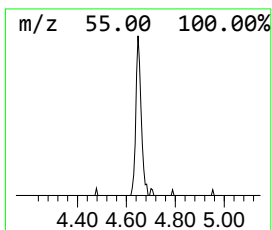
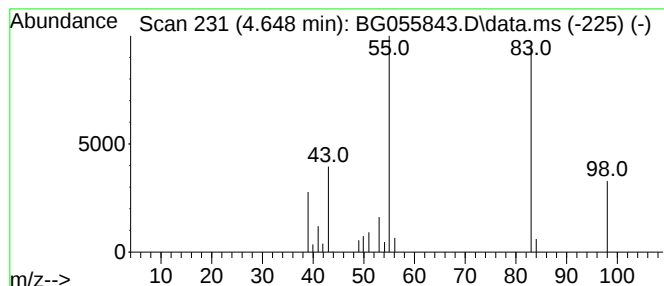
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.648	2.46 ng	24879	1,4-Dichlorobenzene-d4	8.220

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	87
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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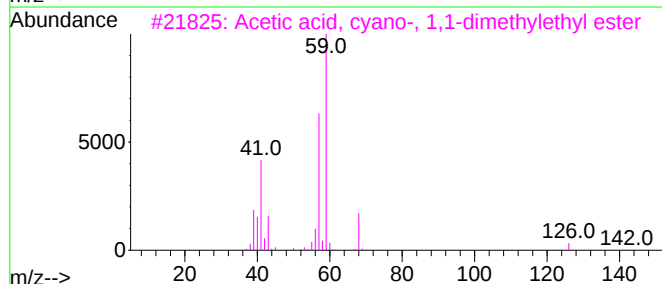
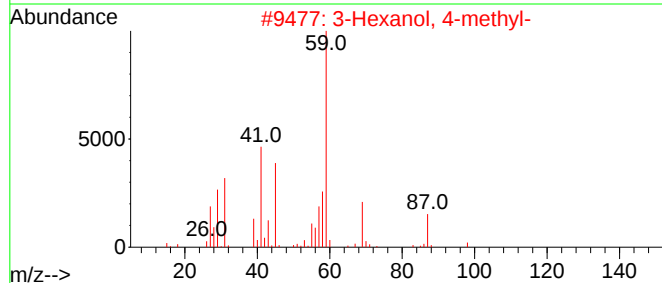
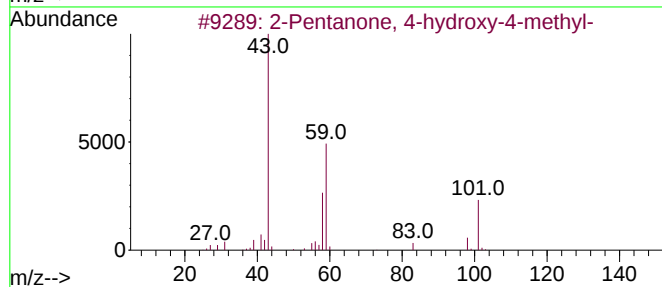
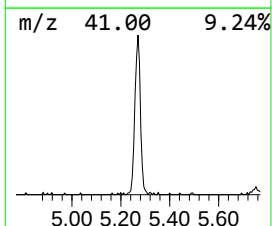
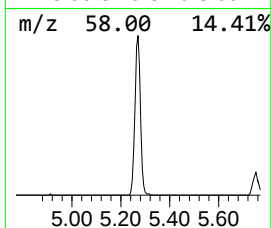
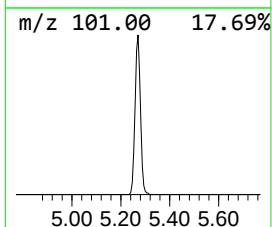
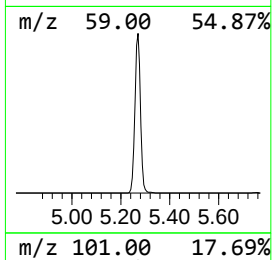
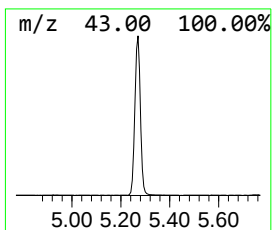
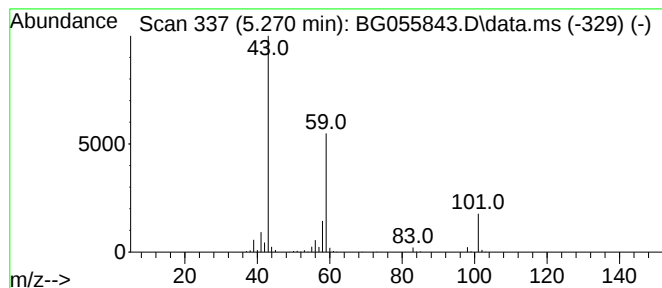
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.270	62.55 ng	632901	1,4-Dichlorobenzene-d4			8.220

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	9



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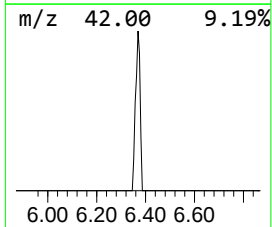
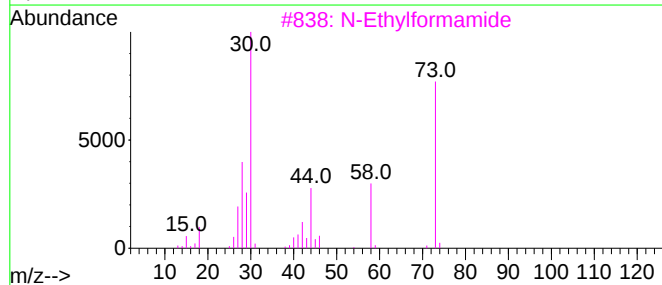
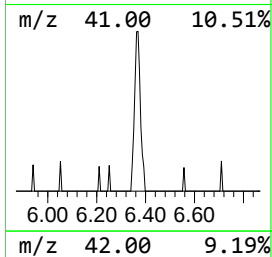
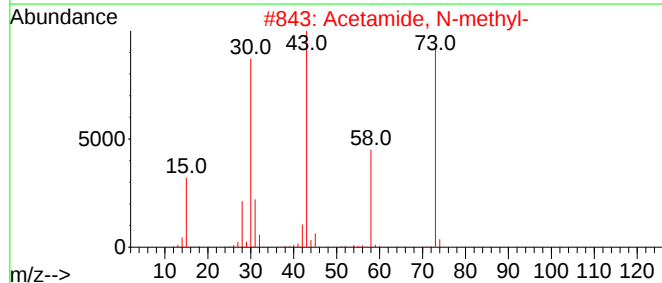
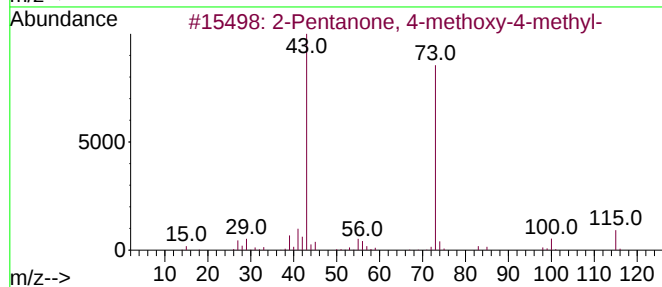
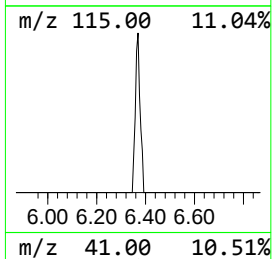
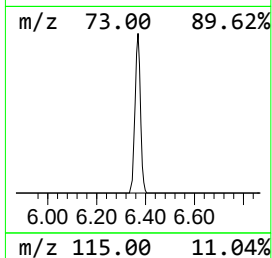
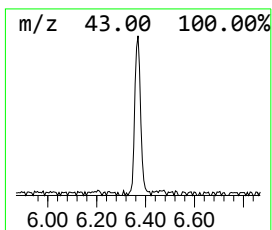
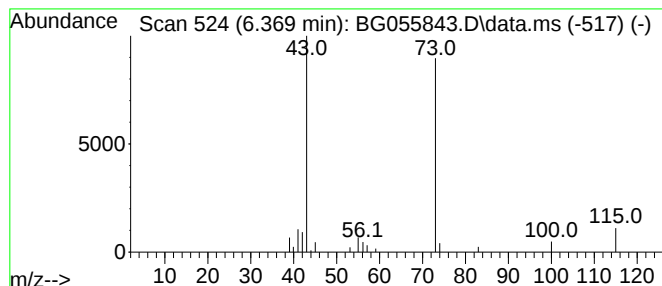
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.369	4.01 ng	40552	1,4-Dichlorobenzene-d4	8.220

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	58
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			Guanidine, methyl-	73	C2H7N3	000471-29-4	9
5			3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	9



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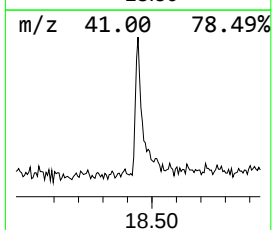
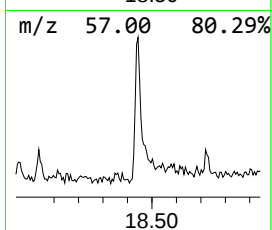
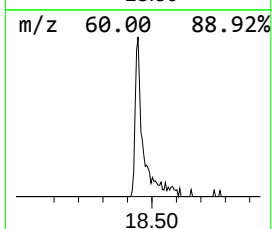
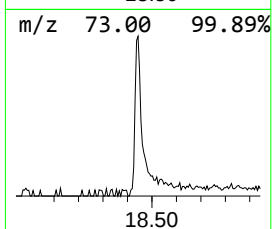
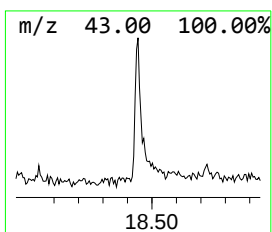
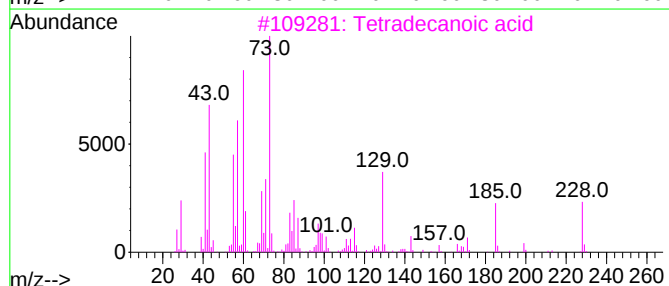
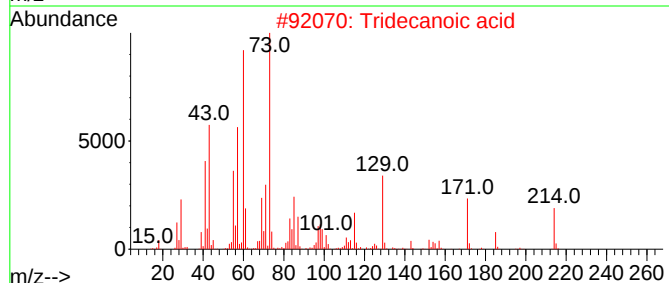
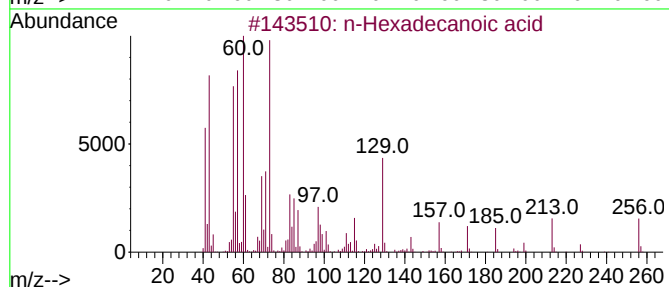
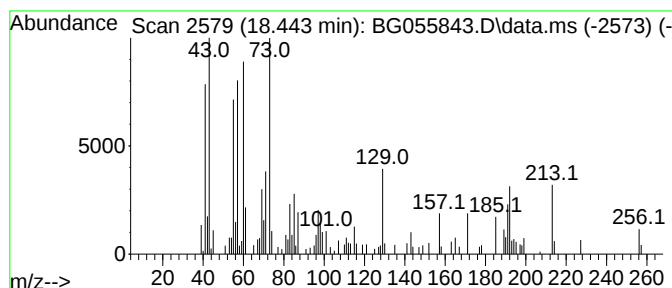
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.443	3.87 ng	117511	Phenanthrene-d10	17.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	52
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.648	2.5	ng	24879	1	8.220	202357	20.0
2-Pentanone, 4-...	5.270	62.5	ng	632901	1	8.220	202357	20.0
2-Pentanone, 4-...	6.369	4.0	ng	40552	1	8.220	202357	20.0
n-Hexadecanoic ...	18.443	3.9	ng	117511	4	17.585	607925	20.0