

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
 Data File : BG049825.D
 Acq On : 12 Aug 2021 19:57
 Operator : CG/JU
 Sample : M3331-12
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BSY1-SB-121314-0-3

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_G\Methods\8270-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.138	12	17	23	rBV	63101	111289	6.77%	1.123%
2	5.112	348	353	362	rVB	29579	50143	3.05%	0.506%
3	5.588	427	434	450	rBV	525265	903052	54.97%	9.110%
4	7.203	699	709	722	rBV	567877	1009853	61.47%	10.187%
5	8.037	843	851	857	rBV	137451	241183	14.68%	2.433%
6	9.206	1041	1050	1058	rBV	370190	668163	40.67%	6.740%
7	10.616	1281	1290	1296	rBV3	40775	77436	4.71%	0.781%
8	10.857	1324	1331	1337	rBV	190465	331770	20.20%	3.347%
9	12.514	1607	1613	1620	rVB3	9459	16991	1.03%	0.171%
10	13.307	1740	1748	1757	rBV	946507	1459758	88.86%	14.726%
11	14.687	1973	1983	1990	rBV	272975	454147	27.65%	4.581%
12	16.185	2231	2238	2244	rBV	705199	1122099	68.31%	11.320%
13	17.442	2446	2452	2457	rBV	313295	477622	29.08%	4.818%
14	17.483	2457	2459	2466	rVB2	23461	31462	1.92%	0.317%
15	18.088	2558	2562	2567	rBV6	12559	17613	1.07%	0.178%
16	18.318	2598	2601	2606	rBV7	18961	27754	1.69%	0.280%
17	18.864	2689	2694	2697	rBV7	12567	21230	1.29%	0.214%
18	19.492	2797	2801	2807	rVB	79063	117581	7.16%	1.186%
19	19.857	2859	2863	2870	rVB	74782	122706	7.47%	1.238%
20	20.050	2889	2896	2902	rBV	1258762	1642719	100.00%	16.572%
21	20.726	3007	3011	3016	rVB	76339	97856	5.96%	0.987%
22	21.349	3115	3117	3122	rVB6	28482	34532	2.10%	0.348%
23	21.725	3175	3181	3188	rBV2	251394	476272	28.99%	4.805%
24	25.008	3733	3740	3753	rVB3	130570	399530	24.32%	4.030%

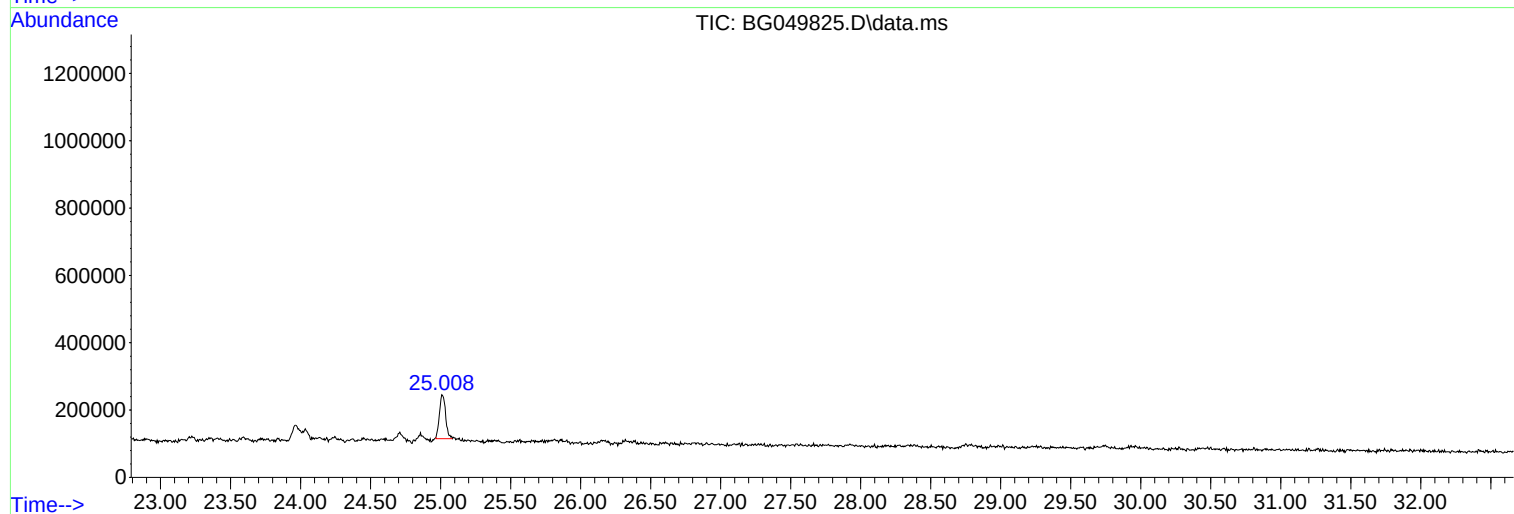
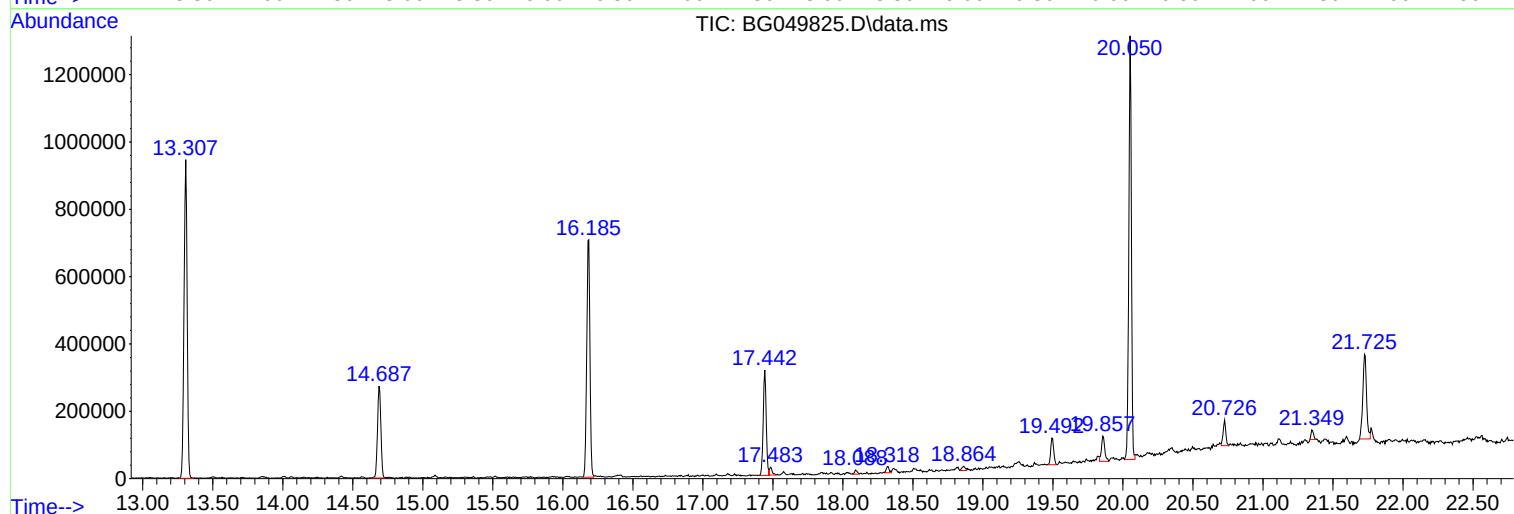
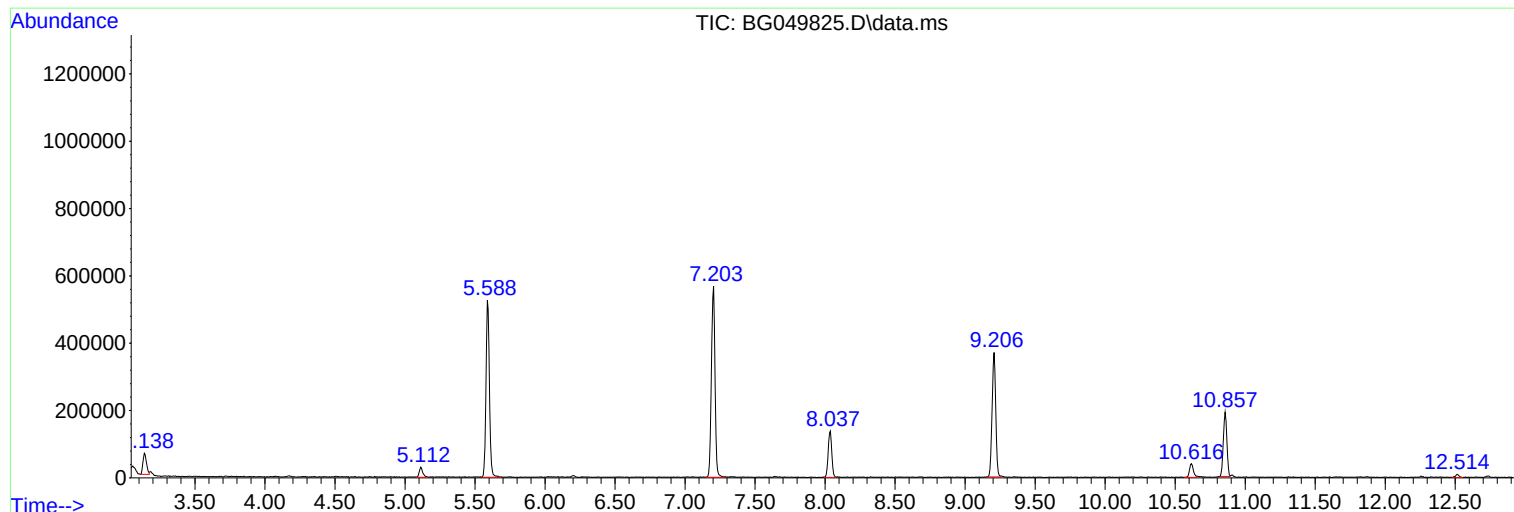
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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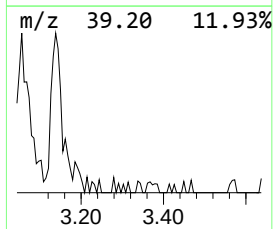
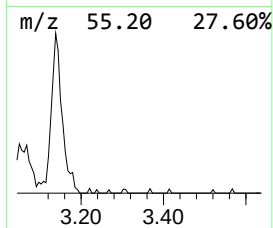
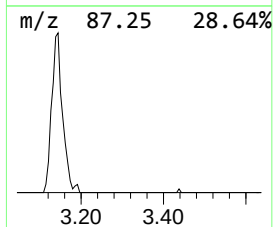
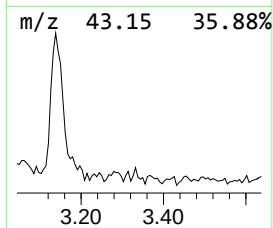
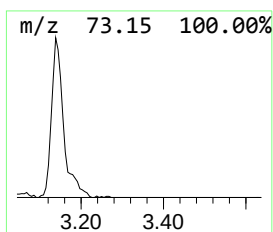
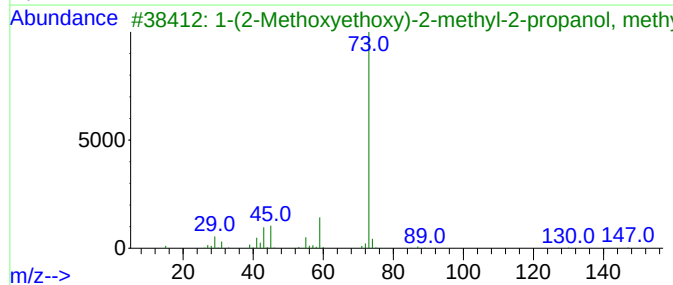
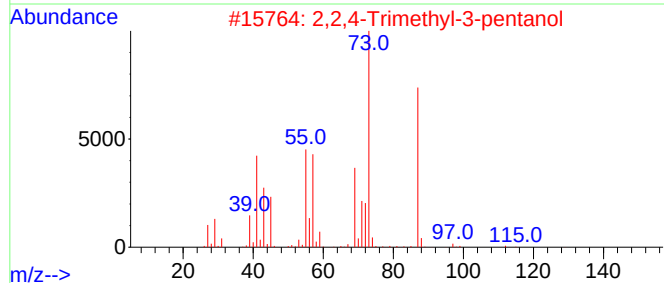
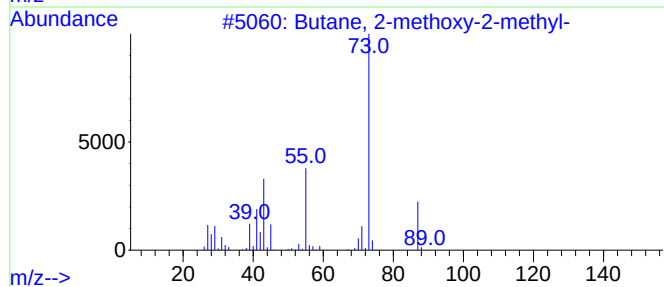
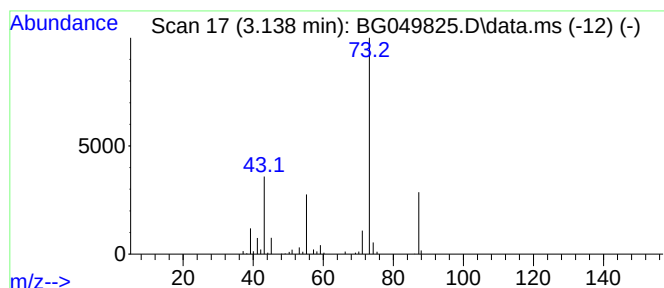
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.138	9.23 ng	111289	1,4-Dichlorobenzene-d4	8.037

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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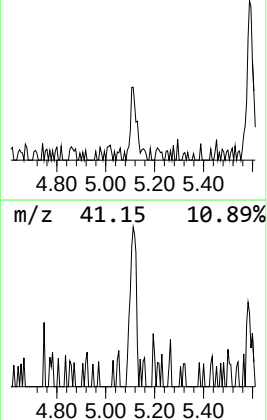
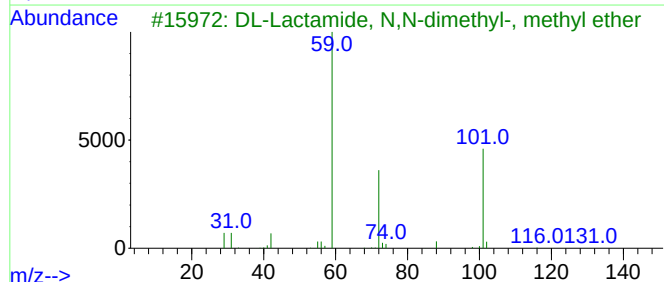
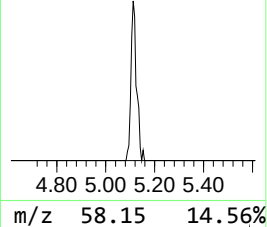
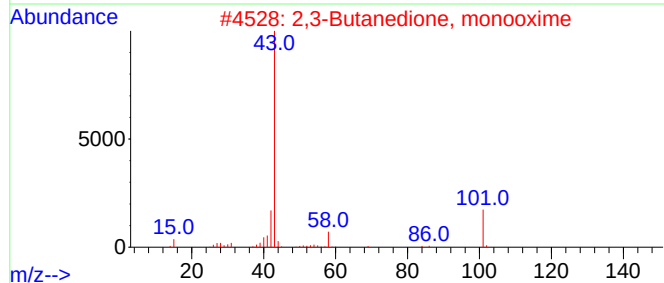
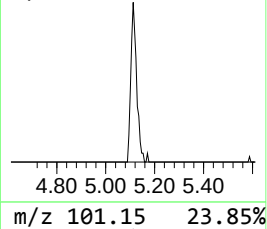
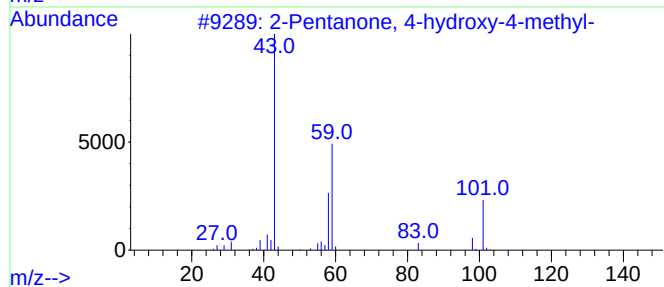
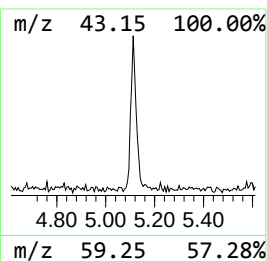
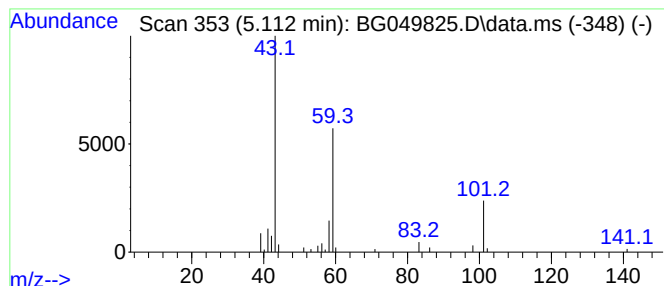
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.112	4.16 ng	50143	1,4-Dichlorobenzene-d4	8.037

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3		DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	37
4		Tetraglyme	222	C10H22O5	000143-24-8	23
5		3-Heptanol	116	C7H16O	000589-82-2	17



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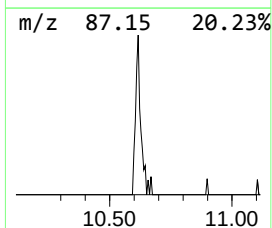
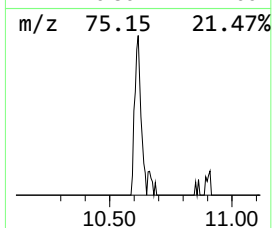
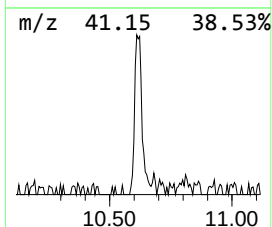
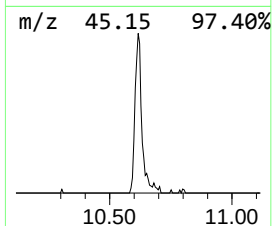
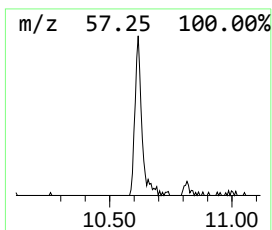
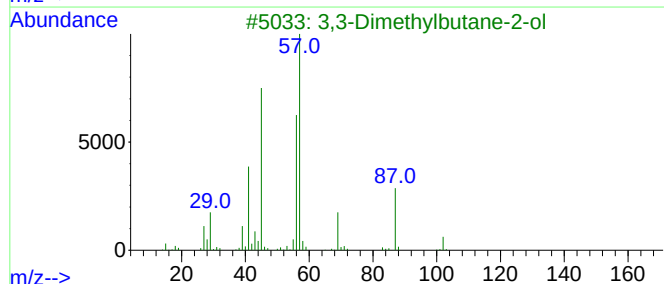
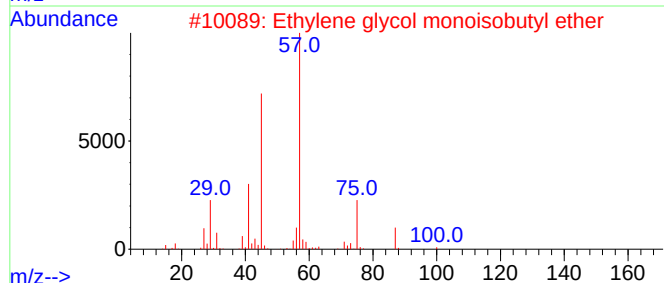
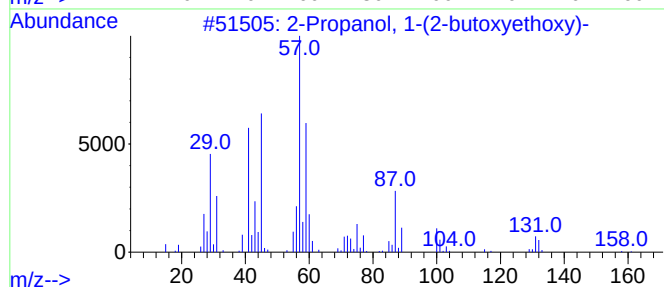
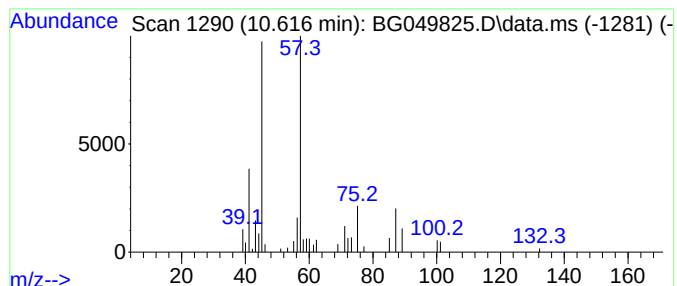
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Peak Number 3 2-Propanol, 1-(2-butoxyetho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.616	4.67 ng	77436	Naphthalene-d8	10.857	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	64
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	53
5	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	47



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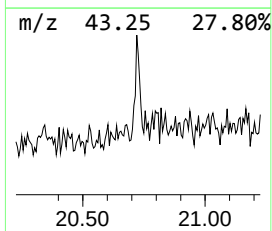
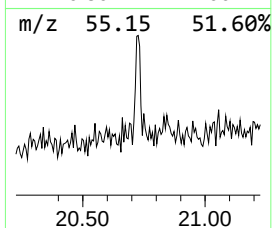
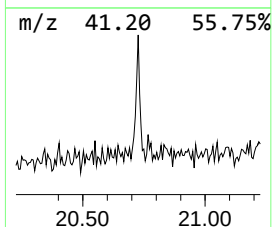
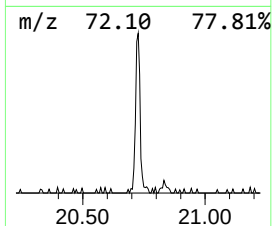
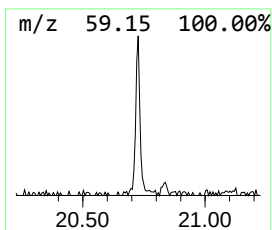
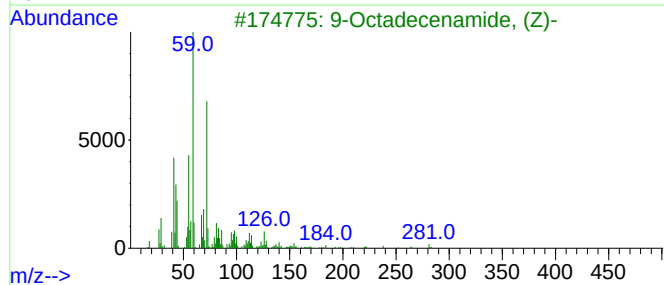
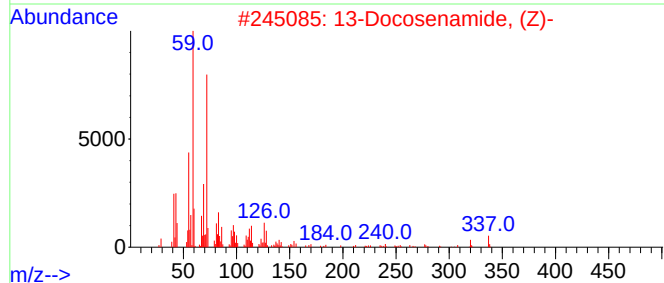
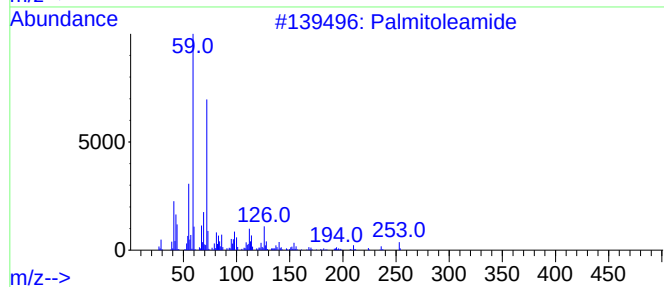
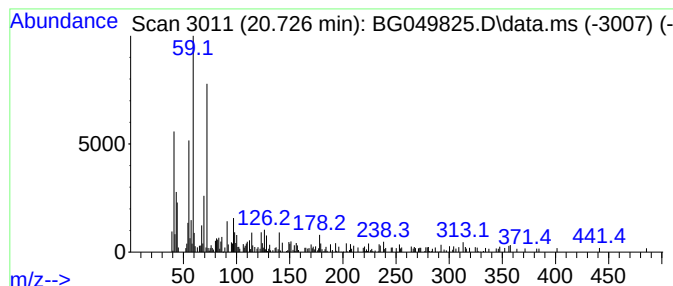
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Peak Number 4 Palmitoleamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.726	4.11 ng	97856	Chrysene-d12	21.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Palmitoleamide	253	C16H31NO	106010-22-4	87
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
4			Dodecanamide	199	C12H25NO	001120-16-7	43
5			Octanamide	143	C8H17NO	000629-01-6	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.138	9.2	ng	111289	1	8.037	241183	20.0
2-Pentanone, 4-...	5.112	4.2	ng	50143	1	8.037	241183	20.0
2-Propanol, 1-(...	10.616	4.7	ng	77436	2	10.857	331770	20.0
Palmitoleamide	20.726	4.1	ng	97856	5	21.725	476272	20.0