

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041323\
 Data File : BG057083.D
 Acq On : 13 Apr 2023 15:39
 Operator : CG/JU
 Sample : PB152099BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB152099BL

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057083.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.431	315	322	329	rBV	128082	193041	12.35%	3.054%
2	5.912	398	404	414	rVB	319005	496583	31.77%	7.856%
3	7.540	673	681	691	rBV	309567	538523	34.45%	8.519%
4	8.403	822	828	835	rBV	52261	86990	5.57%	1.376%
5	9.584	1021	1029	1038	rBV	183580	321560	20.57%	5.087%
6	11.246	1305	1312	1320	rBV	68137	121099	7.75%	1.916%
7	13.643	1713	1720	1728	rBV	515852	823454	52.68%	13.027%
8	15.018	1947	1954	1961	rBV	123539	198496	12.70%	3.140%
9	16.498	2199	2206	2217	rBV	478257	691622	44.25%	10.942%
10	17.761	2414	2421	2430	rVB	180750	278762	17.83%	4.410%
11	20.328	2852	2858	2864	rBV	1232801	1563081	100.00%	24.728%
12	22.073	3149	3155	3164	rVB2	177211	299562	19.16%	4.739%
13	23.641	3415	3422	3427	rVB3	17785	33566	2.15%	0.531%
14	24.522	3566	3572	3578	rVB5	22622	47352	3.03%	0.749%
15	25.609	3743	3757	3769	rVB3	93625	367603	23.52%	5.816%
16	26.819	3953	3963	3974	rVB4	32463	105409	6.74%	1.668%
17	28.323	4208	4219	4231	rVB3	28666	103641	6.63%	1.640%
18	30.127	4520	4526	4527	rBV5	11928	17417	1.11%	0.276%
19	32.324	4890	4900	4903	rBV5	12403	33310	2.13%	0.527%

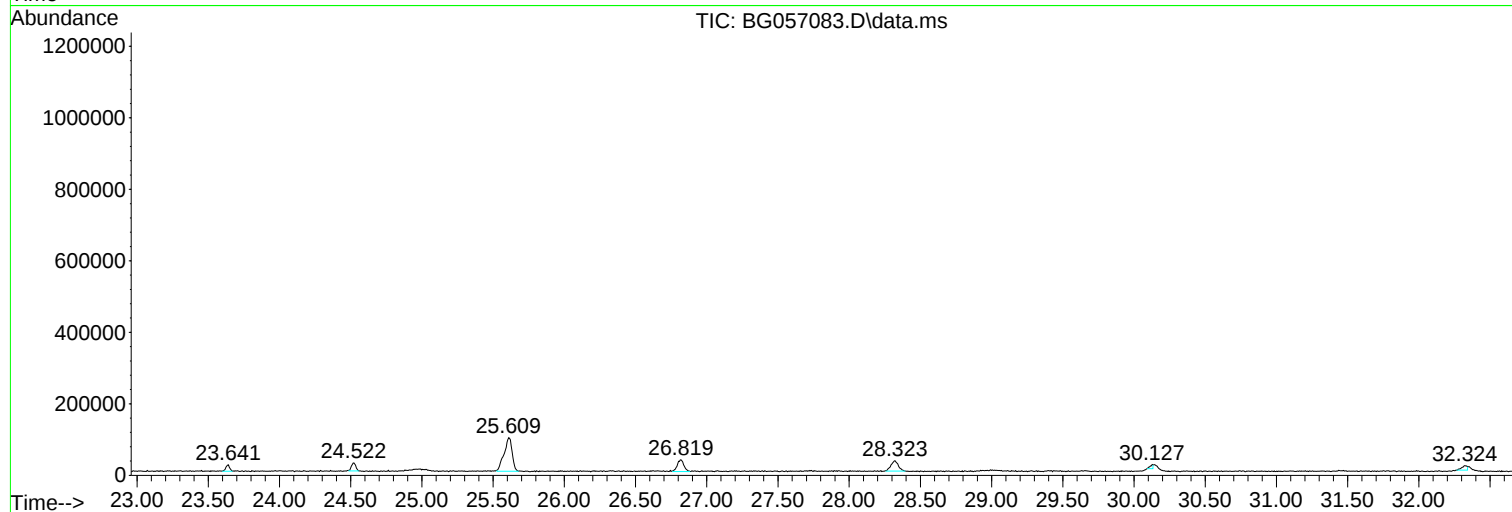
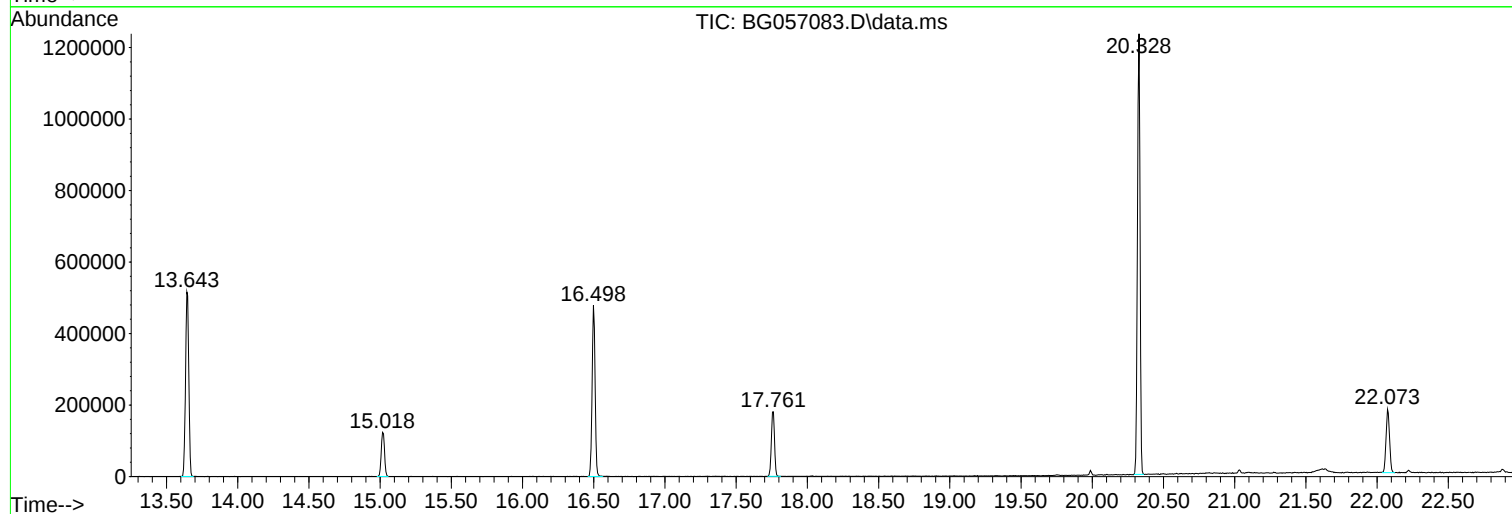
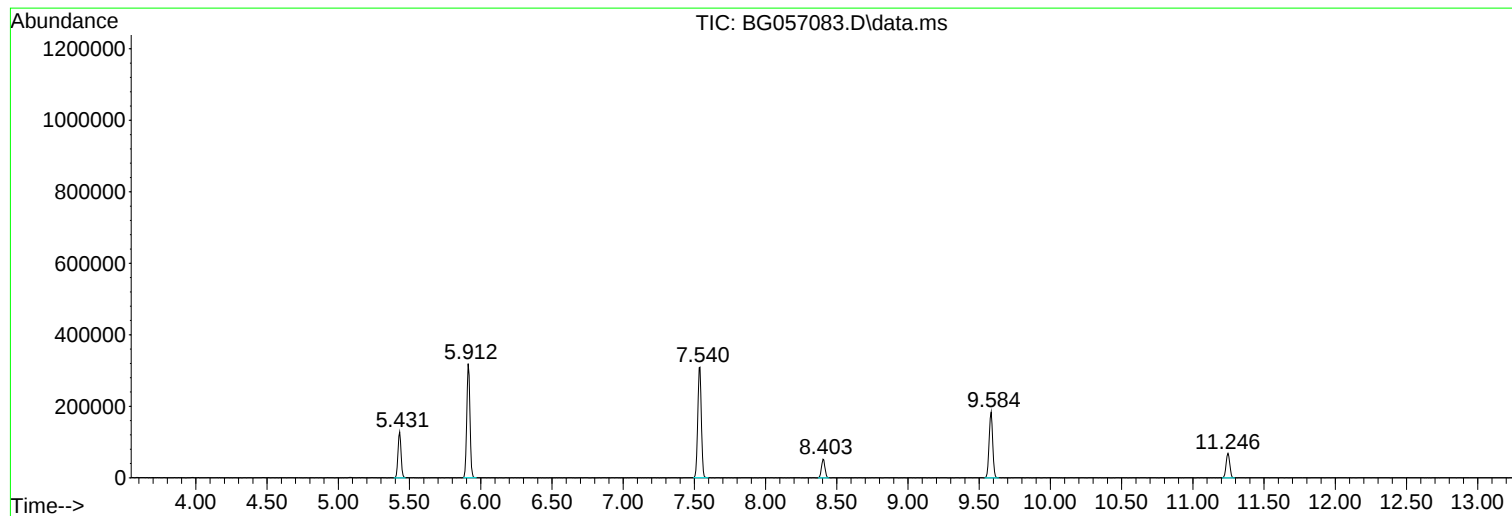
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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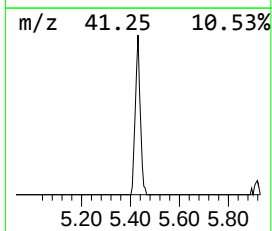
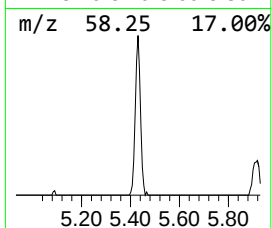
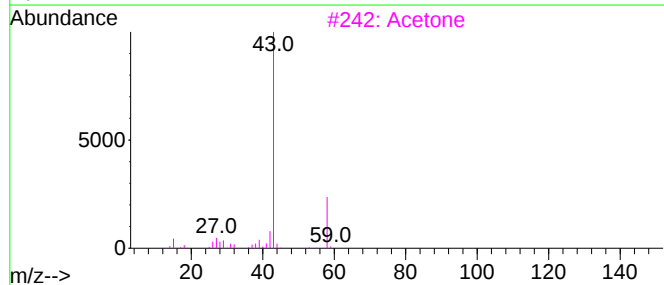
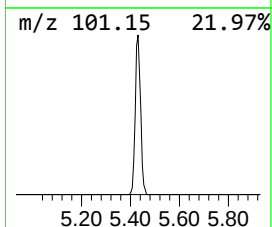
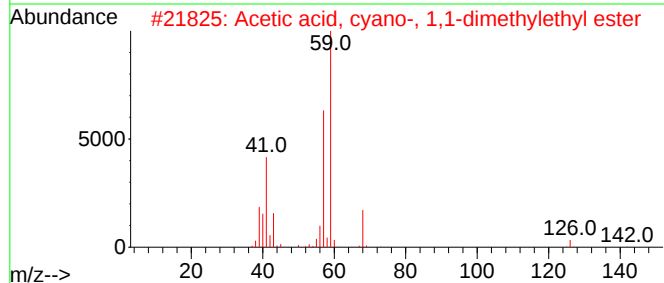
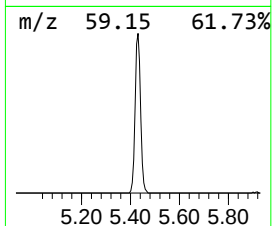
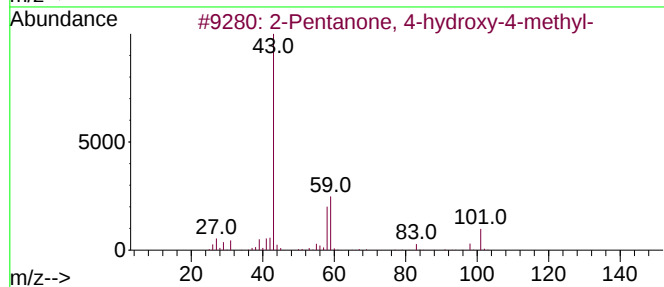
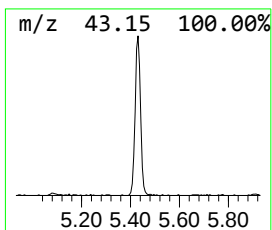
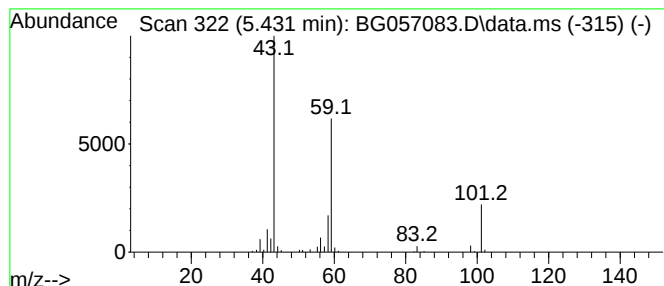
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.431	44.38 ng	193041	1,4-Dichlorobenzene-d4	8.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			Acetone	58	C3H6O	000067-64-1	14
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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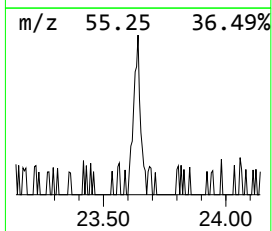
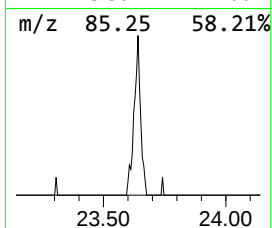
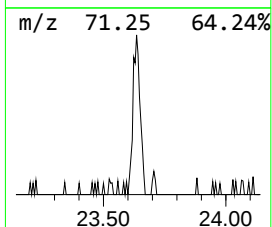
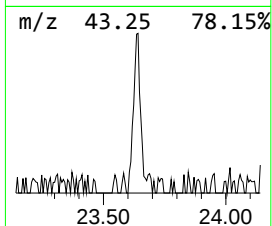
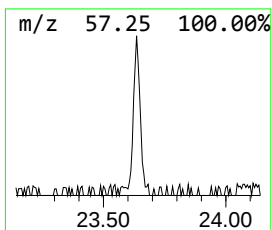
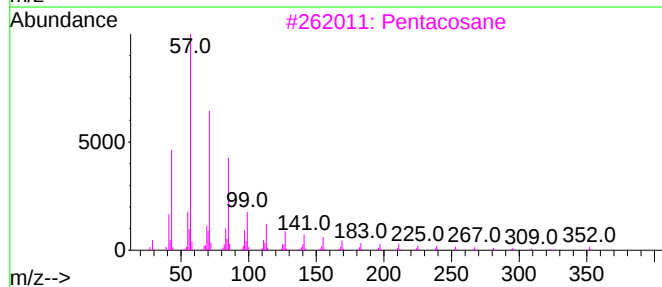
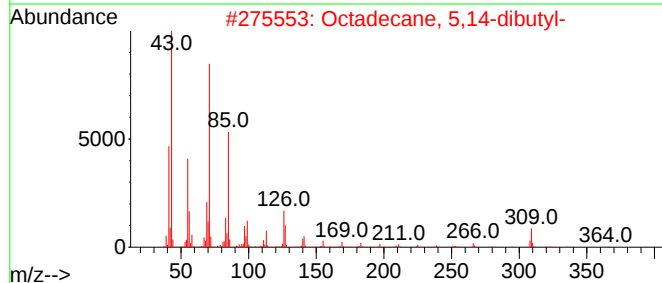
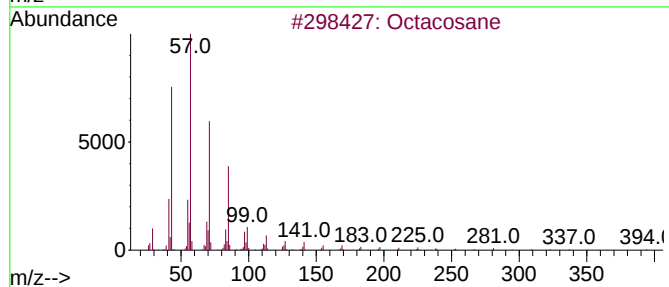
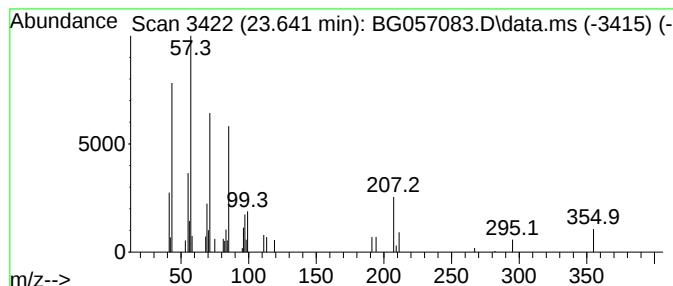
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.641	2.24 ng	33566	Chrysene-d12	22.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	52
2			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	47
3			Pentacosane	352	C25H52	000629-99-2	47
4			1-Iodoundecane	282	C11H23I	004282-44-4	46
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	43



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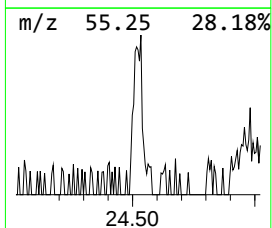
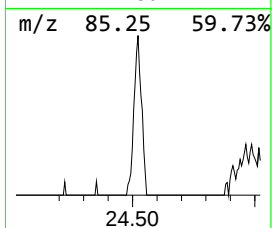
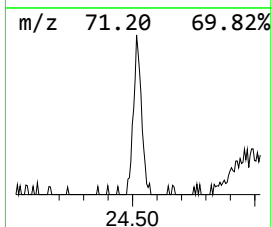
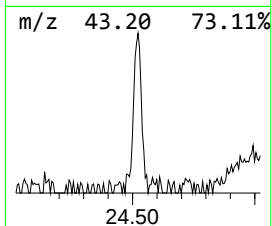
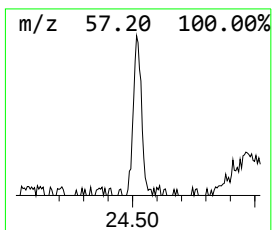
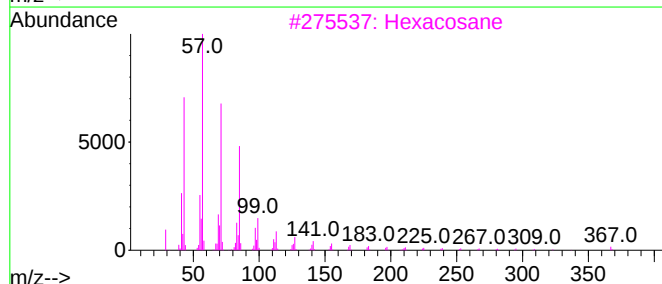
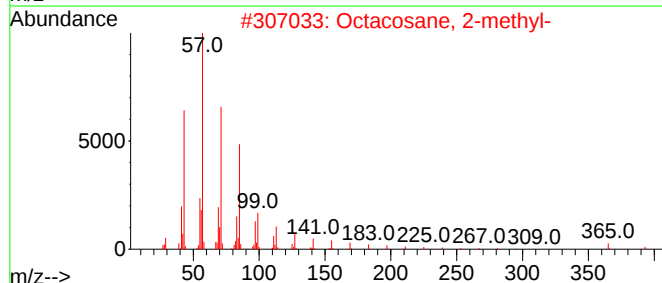
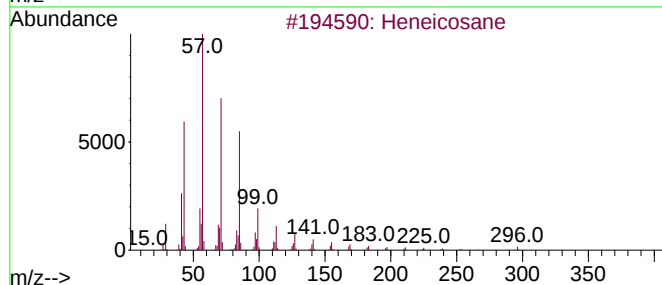
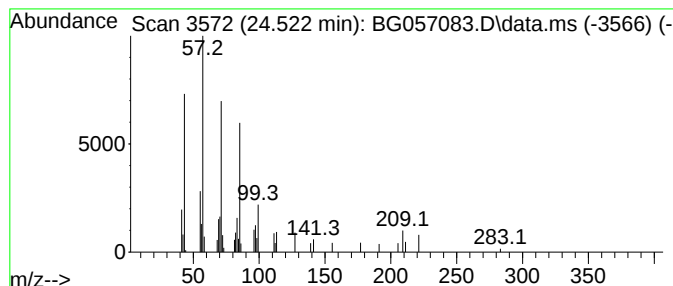
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Peak Number 3 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.523	2.58 ng	47352	Perylene-d12	25.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	83
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	80
3			Hexacosane	366	C26H54	000630-01-3	74
4			Tetracosane	338	C24H50	000646-31-1	72
5			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	72



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ClientSampleId :
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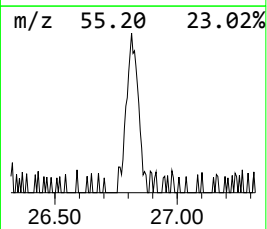
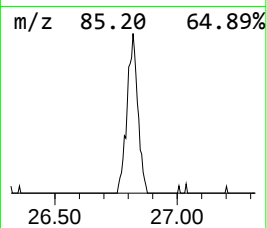
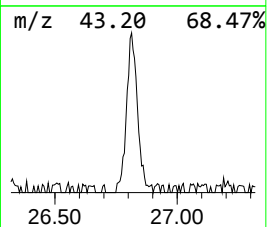
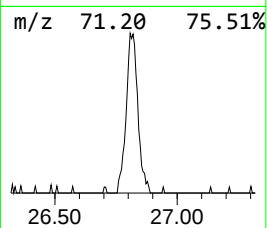
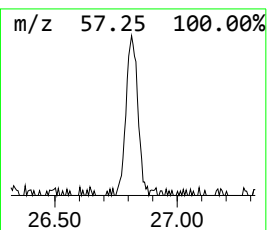
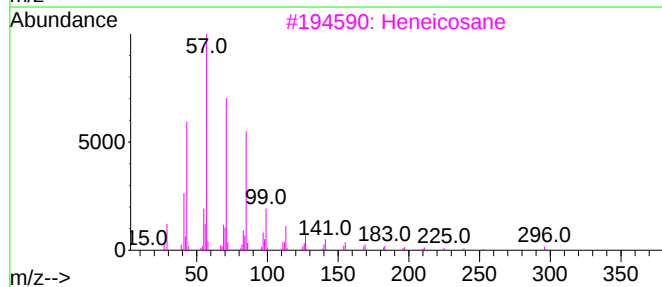
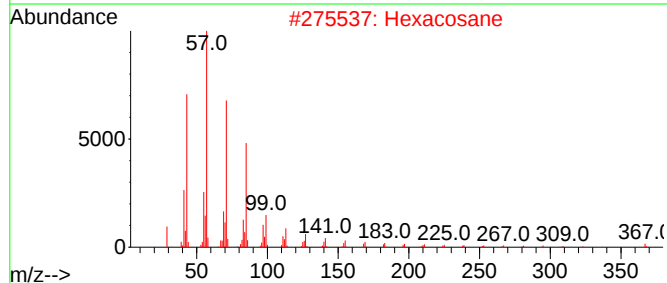
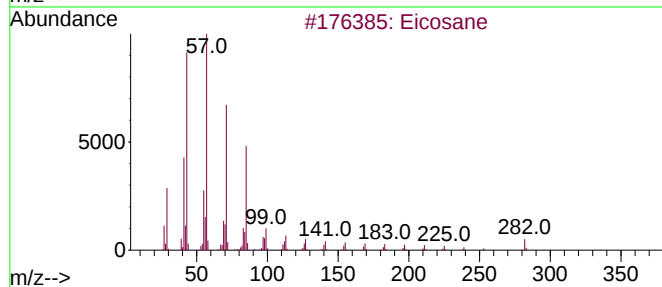
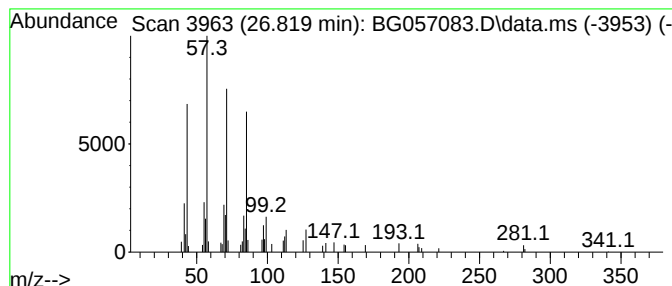
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Peak Number 4 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.819	5.73 ng	105409	Perylene-d12	25.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	94
2	Hexacosane			366	C26H54	000630-01-3	91
3	Heneicosane			296	C21H44	000629-94-7	91
4	Pentacosane			352	C25H52	000629-99-2	91
5	Heneicosane, 11-(1-ethylpropyl)-			366	C26H54	055282-11-6	90



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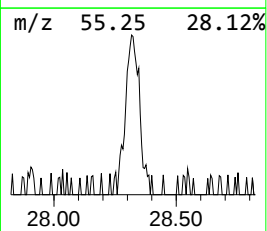
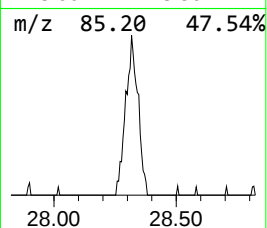
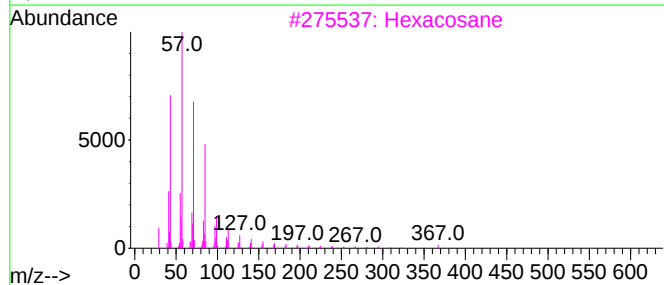
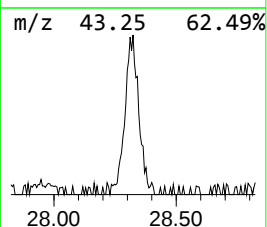
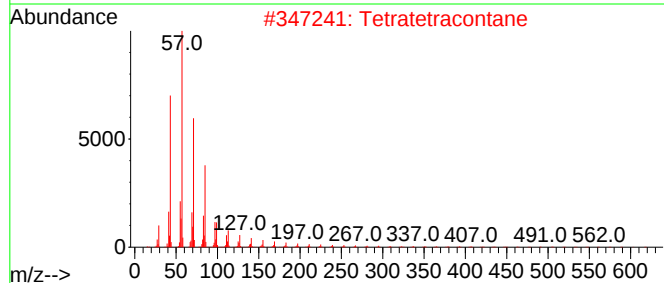
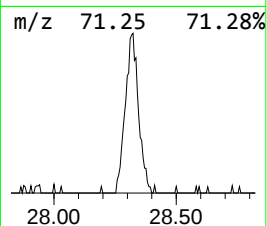
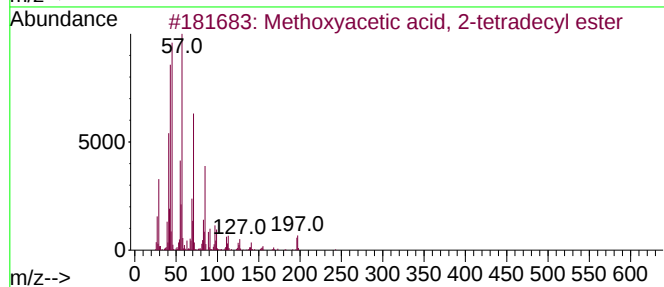
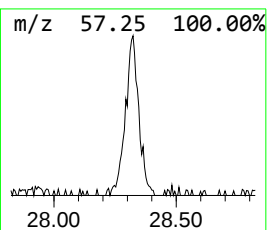
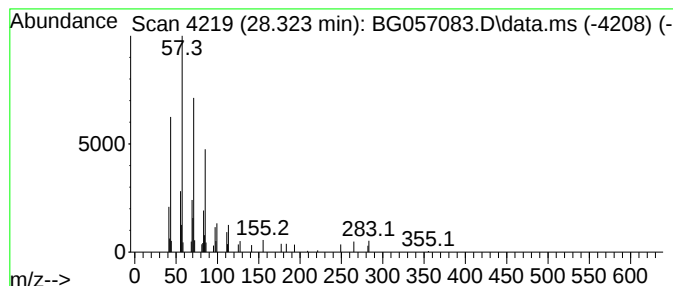
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Peak Number 5 Methoxyacetic acid, 2-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.323	5.64 ng	103641	Perylene-d12	25.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	91
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Hexacosane	366	C26H54	000630-01-3	83
4			Hentriacontane	437	C31H64	000630-04-6	83
5			Tetracosane	338	C24H50	000646-31-1	80



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.431	44.4	ng	193041	1	8.403	86990	20.0
Octacosane	23.641	2.2	ng	33566	5	22.073	299562	20.0
Heneicosane	24.523	2.6	ng	47352	6	25.615	367603	20.0
Eicosane	26.819	5.7	ng	105409	6	25.615	367603	20.0
Methoxyacetic a...	28.323	5.6	ng	103641	6	25.615	367603	20.0