

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042423\
 Data File : BF132994.D
 Acq On : 24 Apr 2023 14:35
 Operator : CG\JU
 Sample : 02468-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUMP-PUMP-GW-SAMPLE

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_F\Methods\8270-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.934	476	484	487	rBV	1334860	1403092	21.03%	3.810%
2	5.351	551	555	559	rBV	2220431	2029240	30.41%	5.511%
3	6.375	725	729	732	rBV	1590915	1235455	18.52%	3.355%
4	6.745	788	792	795	rBV	1709913	1365359	20.46%	3.708%
5	7.310	882	888	891	rBV	4285227	4306297	64.54%	11.695%
6	7.410	898	905	912	rBV	88987	128351	1.92%	0.349%
7	8.028	1006	1010	1013	rBV	2363265	1882025	28.21%	5.111%
8	9.110	1188	1194	1197	rBV	7370174	6671978	100.00%	18.120%
9	9.780	1304	1308	1311	rBV	2577719	2085881	31.26%	5.665%
10	10.492	1426	1429	1432	rBV	184819	139762	2.09%	0.380%
11	10.569	1437	1442	1445	rBV	3276212	2790437	41.82%	7.578%
12	11.263	1556	1560	1563	rBV	2527351	1991356	29.85%	5.408%
13	11.804	1648	1652	1666	rBV	879432	901332	13.51%	2.448%
14	12.586	1782	1785	1799	rVB	537928	557516	8.36%	1.514%
15	12.857	1826	1831	1834	rBV	6168039	6152809	92.22%	16.710%
16	13.786	1985	1989	1998	rVB2	124329	220008	3.30%	0.597%
17	13.898	2004	2008	2011	rBV	1698471	1446457	21.68%	3.928%
18	13.998	2022	2025	2032	rVB	70016	79838	1.20%	0.217%
19	14.757	2150	2154	2159	rVB	217994	208248	3.12%	0.566%
20	15.321	2245	2250	2256	rBV	1078952	1226631	18.38%	3.331%

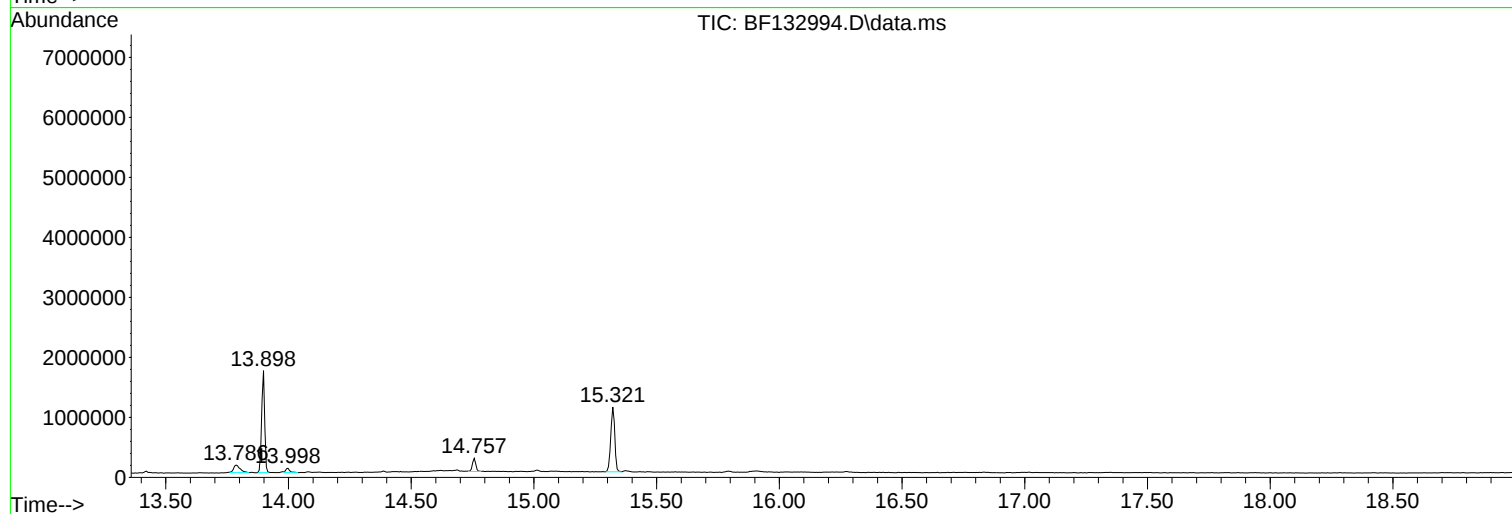
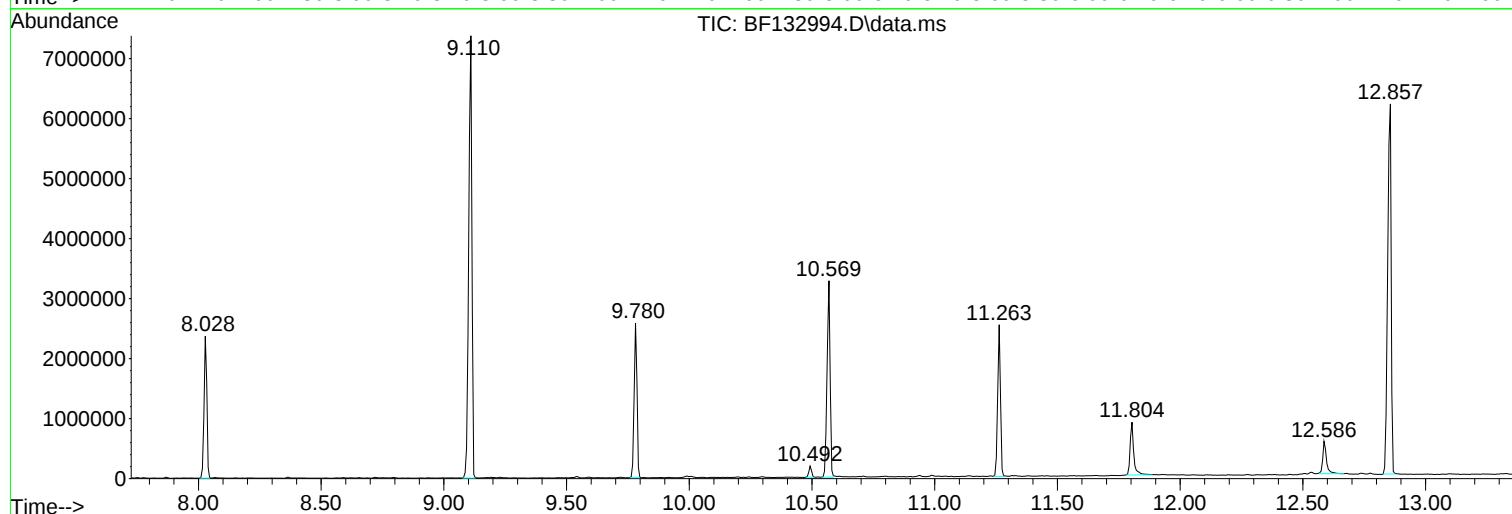
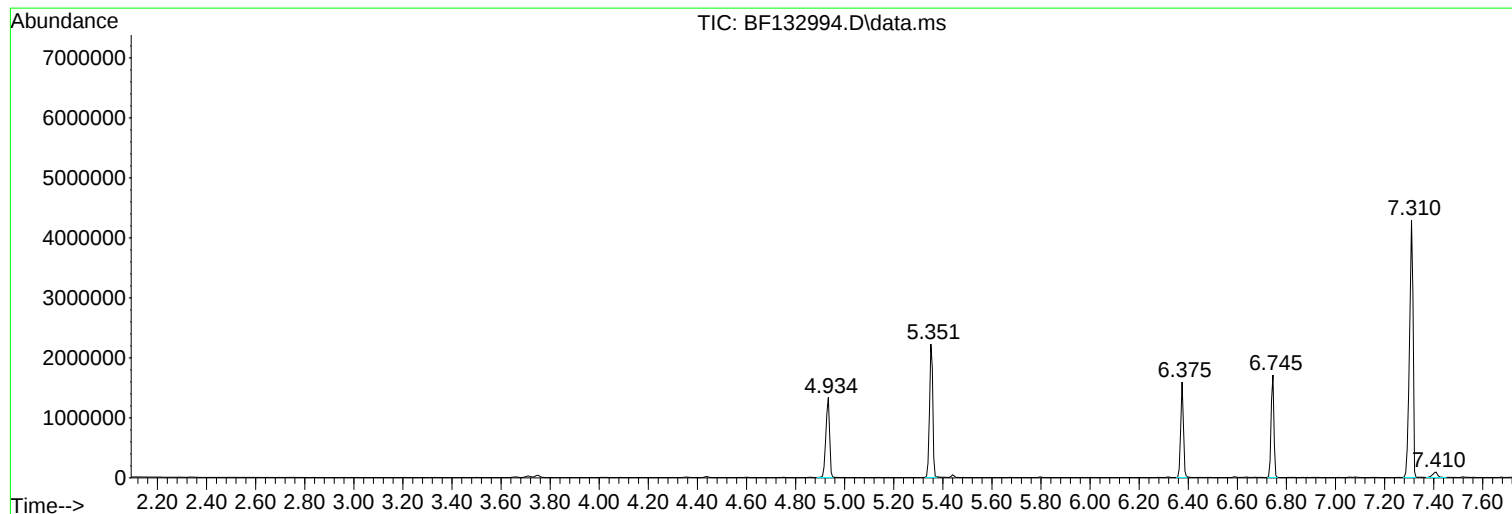
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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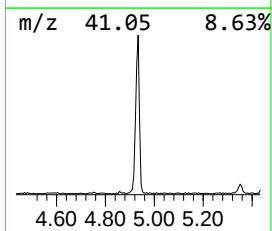
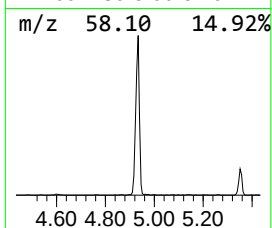
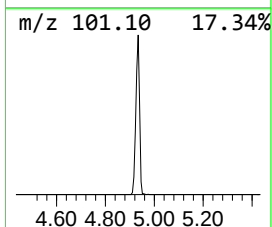
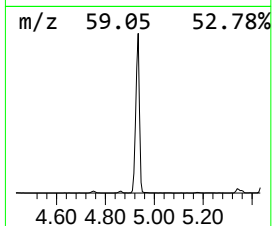
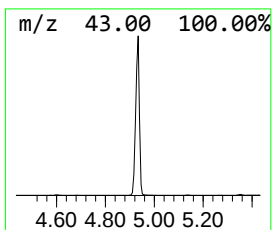
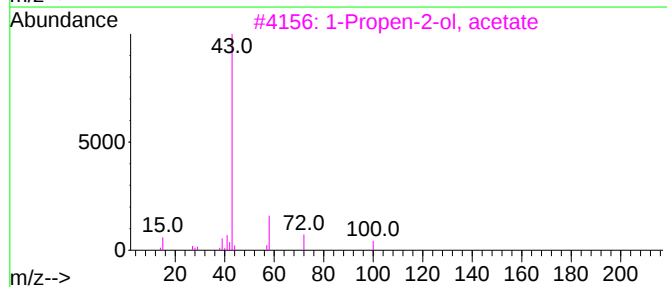
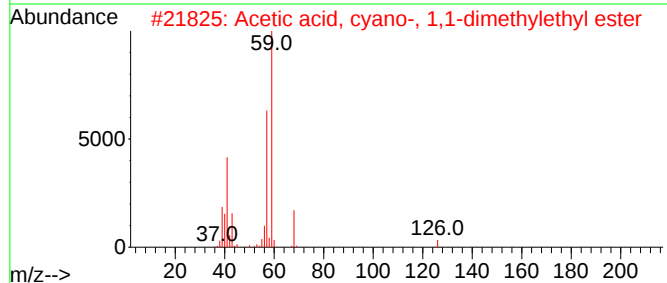
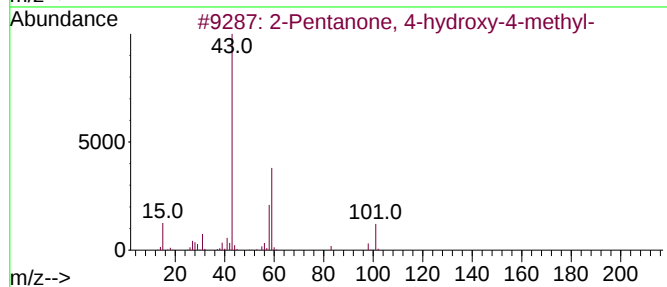
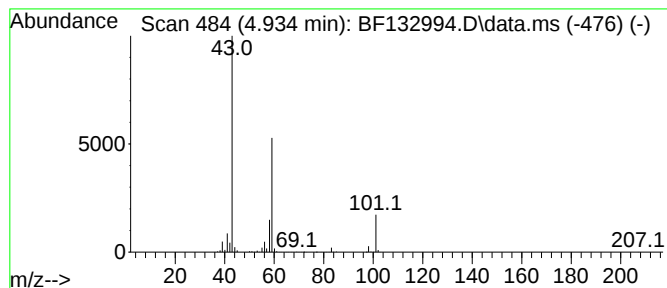
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.934	20.55 ng	1403090	1,4-Dichlorobenzene-d4	6.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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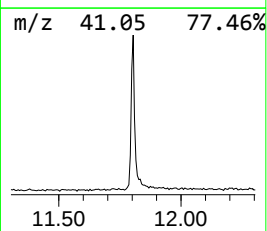
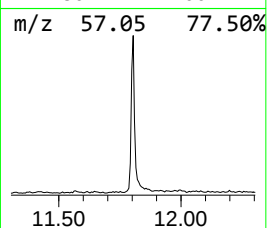
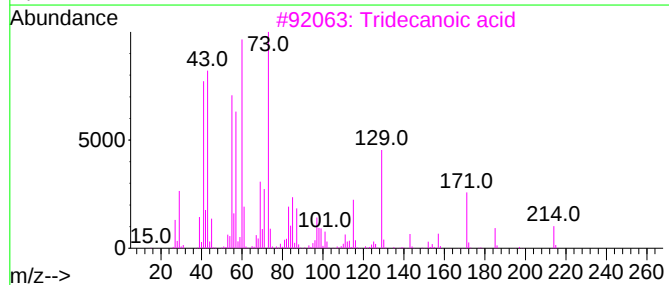
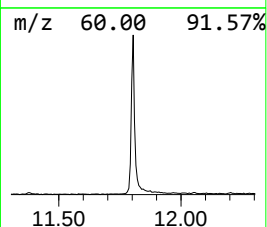
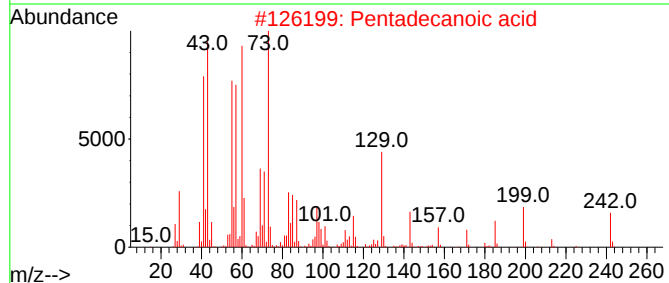
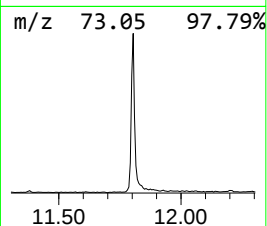
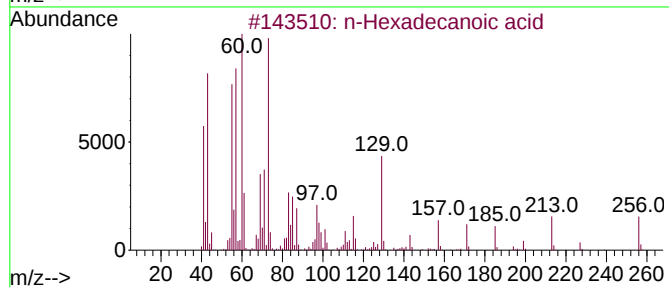
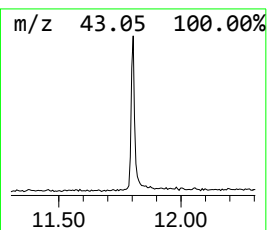
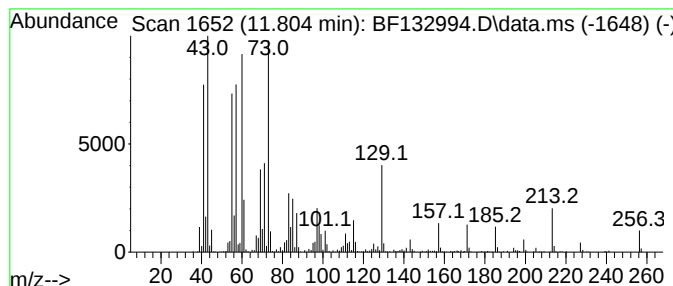
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	9.05 ng	901332	Phenanthrene-d10	11.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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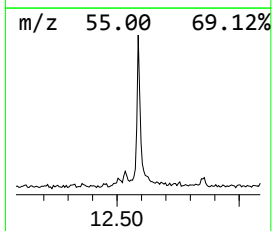
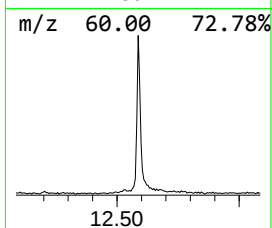
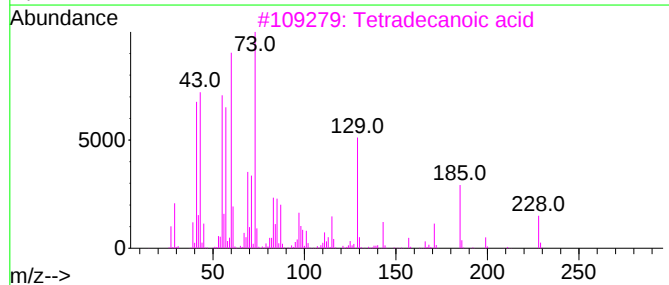
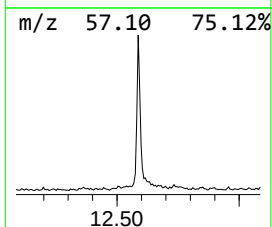
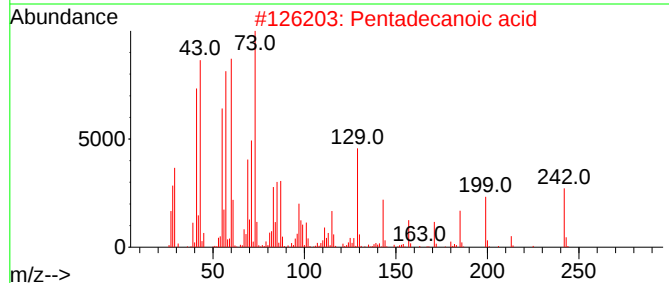
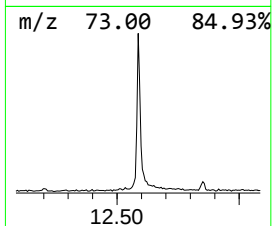
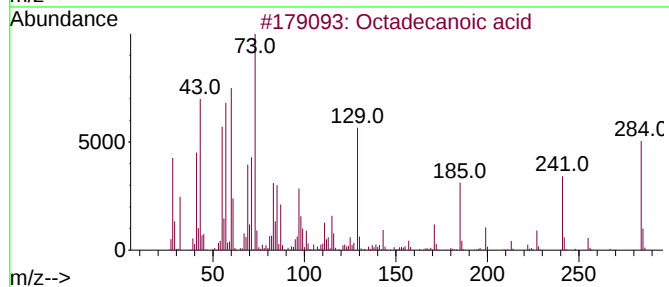
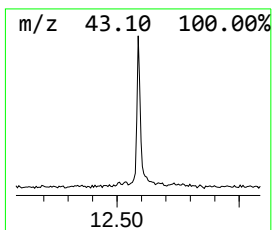
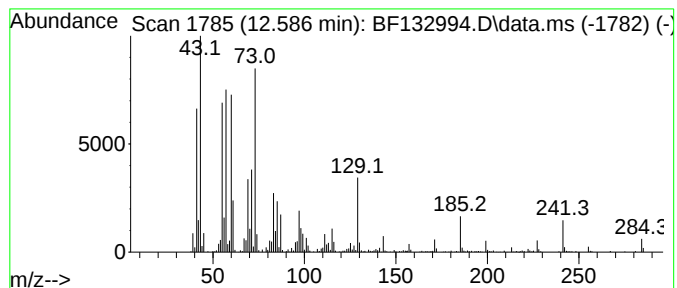
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	7.71 ng	557516	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			n-Decanoic acid	172	C10H20O2	000334-48-5	58
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	38



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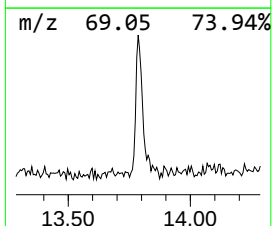
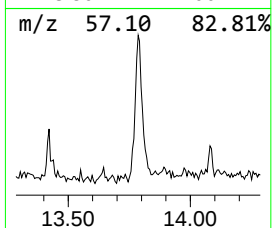
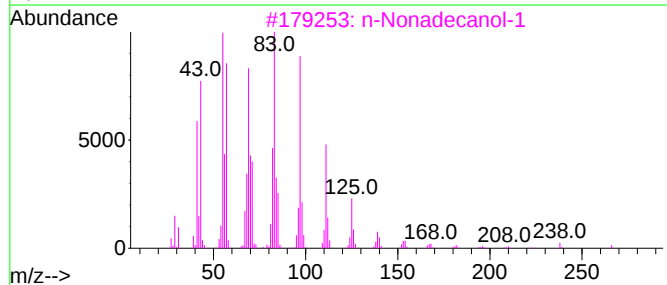
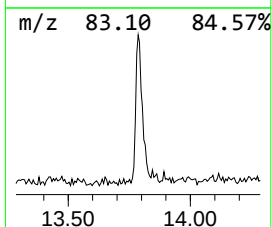
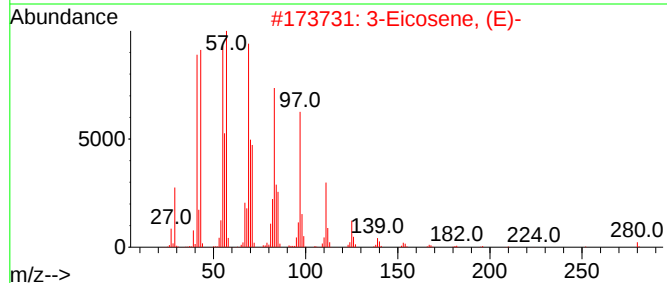
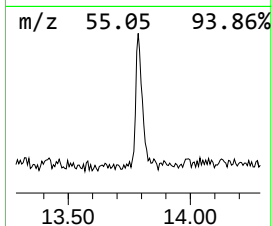
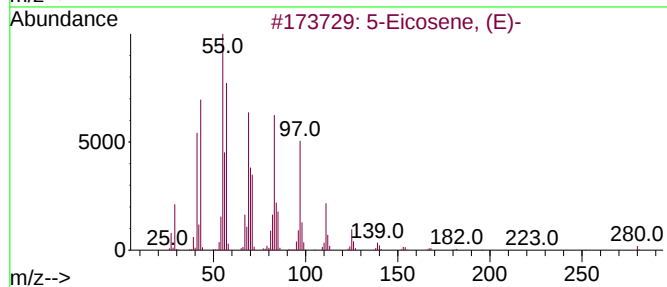
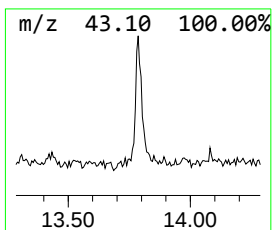
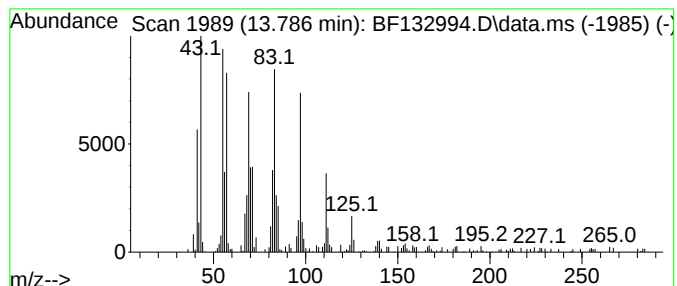
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	3.04 ng	220008	Chrysene-d12	13.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		1-Heneicosanol	312	C21H44O	015594-90-8	95
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	94



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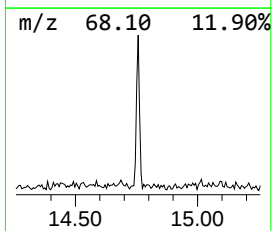
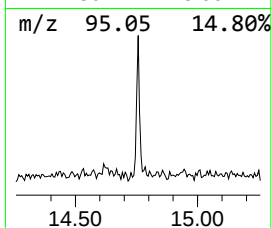
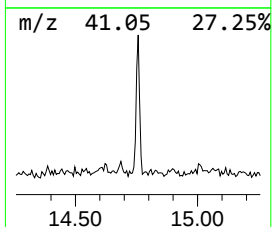
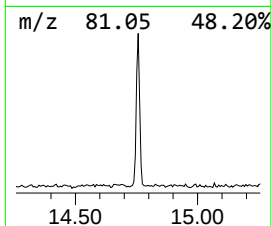
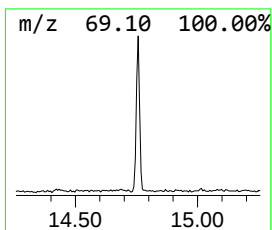
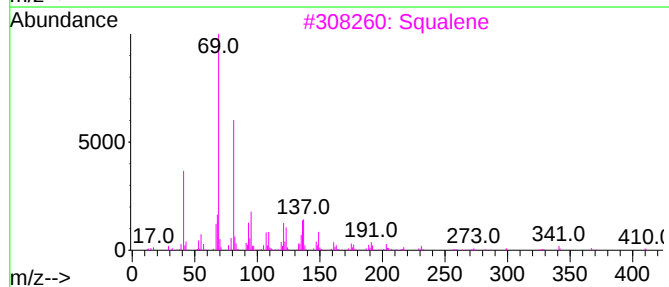
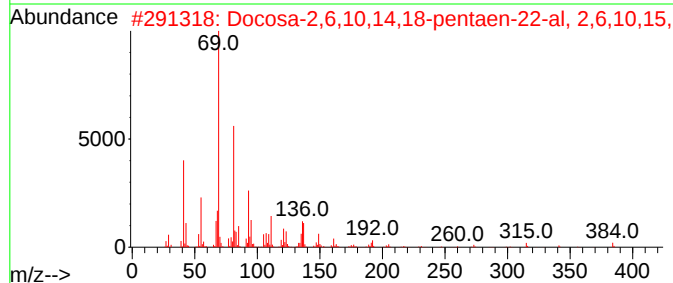
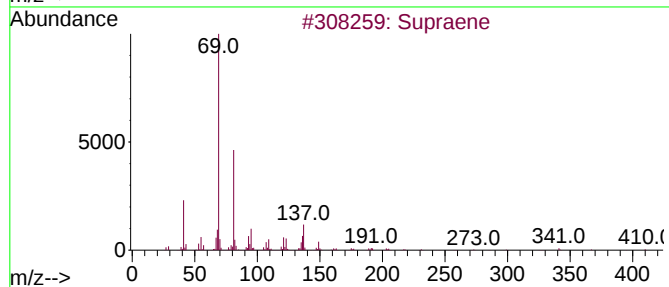
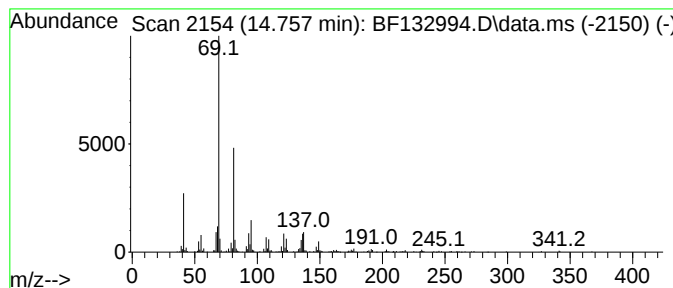
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	3.40 ng	208248	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3			Squalene	410	C30H50	000111-02-4	83
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5			trans-Farnesol	222	C15H26O	000106-28-5	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.934	20.6	ng	1403090	1	6.745	1365360	20.0
n-Hexadecanoic ...	11.804	9.1	ng	901332	4	11.263	1991360	20.0
Octadecanoic acid	12.586	7.7	ng	557516	5	13.898	1446460	20.0
5-Eicosene, (E)-	13.786	3.0	ng	220008	5	13.898	1446460	20.0
Supraene	14.757	3.4	ng	208248	6	15.321	1226630	20.0