

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
 Data File : BF137231.D
 Acq On : 01 Feb 2024 14:51
 Operator : CG\JU
 Sample : P1270-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-LIQUID-20240126

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-BF013024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137231.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	494	497	504	rVB	47753	57757	2.52%	0.521%
2	5.416	563	566	579	rBV	786609	786117	34.28%	7.090%
3	6.416	732	736	746	rBV	500724	451195	19.68%	4.069%
4	6.793	796	800	810	rBV	372320	348810	15.21%	3.146%
5	7.351	889	895	898	rBV	1278109	1229661	53.63%	11.090%
6	8.069	1013	1017	1020	rBV	514854	445780	19.44%	4.021%
7	9.028	1176	1180	1185	rBV2	21110	29568	1.29%	0.267%
8	9.145	1196	1200	1204	rBV	2384046	2293059	100.00%	20.681%
9	9.822	1311	1315	1319	rBV	606181	493783	21.53%	4.453%
10	10.616	1445	1450	1453	rBV	1544021	1370081	59.75%	12.357%
11	11.316	1565	1569	1576	rBV	498438	465448	20.30%	4.198%
12	11.857	1655	1661	1670	rBV2	123488	184635	8.05%	1.665%
13	12.645	1792	1795	1804	rBV2	49062	62960	2.75%	0.568%
14	12.916	1836	1841	1844	rBV	2167170	1955736	85.29%	17.639%
15	13.480	1933	1937	1943	rBV3	17410	25701	1.12%	0.232%
16	13.833	1993	1997	2006	rBV3	27577	42967	1.87%	0.388%
17	13.969	2015	2020	2027	rBV	364325	372514	16.25%	3.360%
18	14.851	2166	2170	2175	rVB	92558	101758	4.44%	0.918%
19	15.121	2210	2216	2221	rVB6	15219	28896	1.26%	0.261%
20	15.445	2264	2271	2278	rBV	247115	341119	14.88%	3.077%

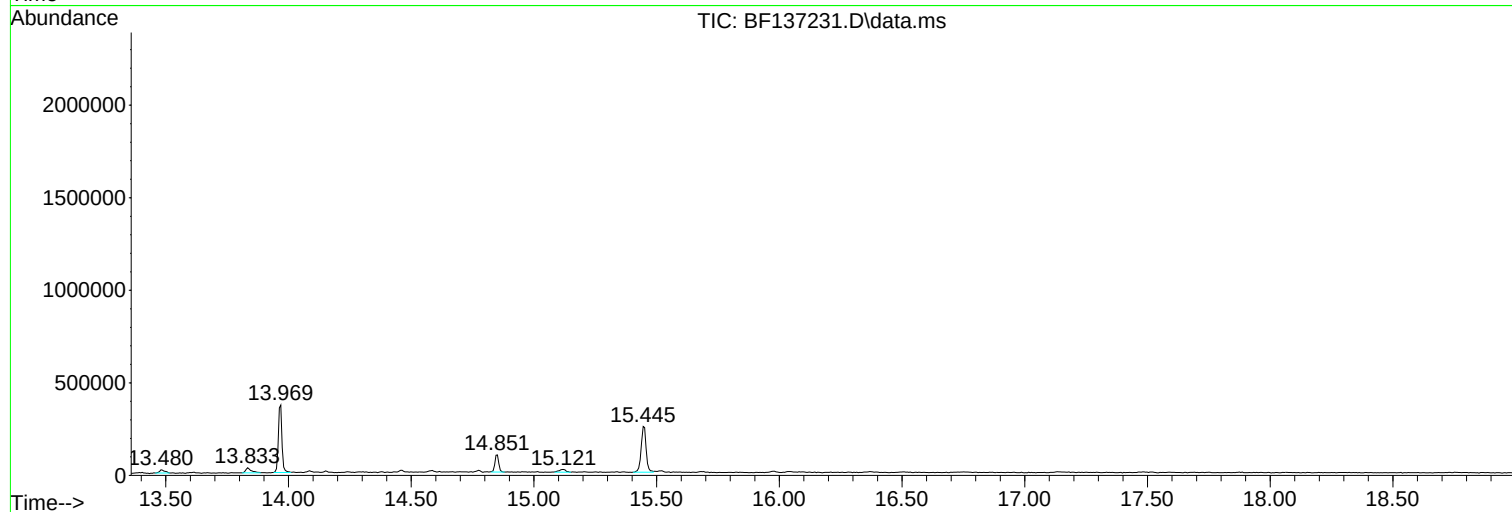
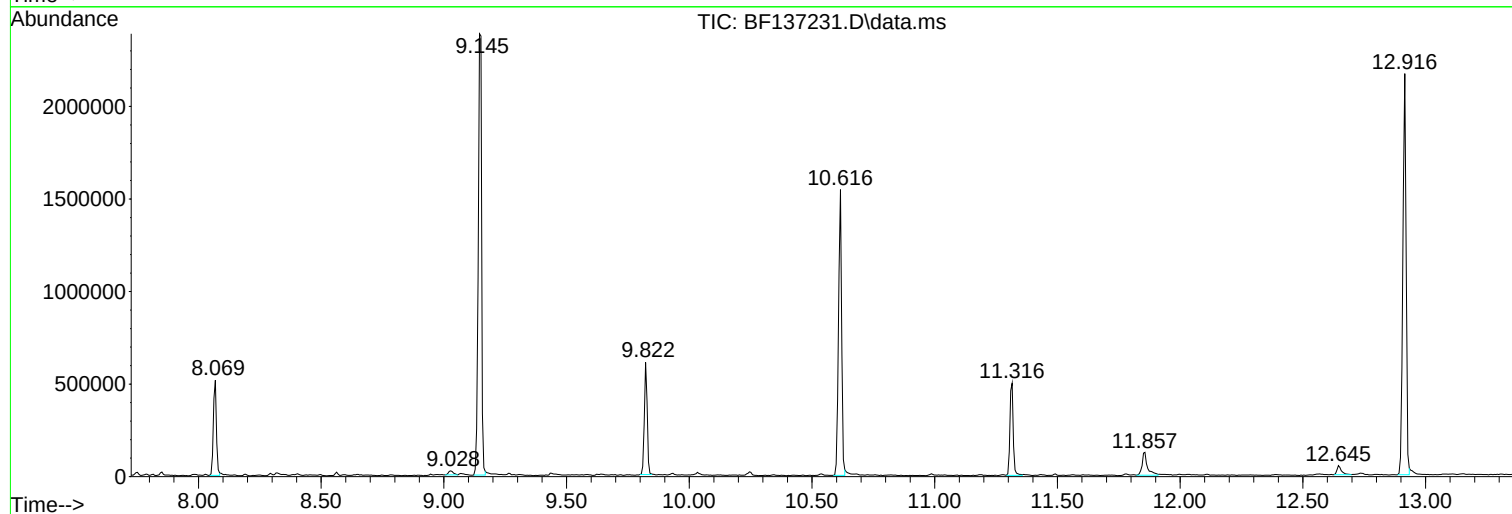
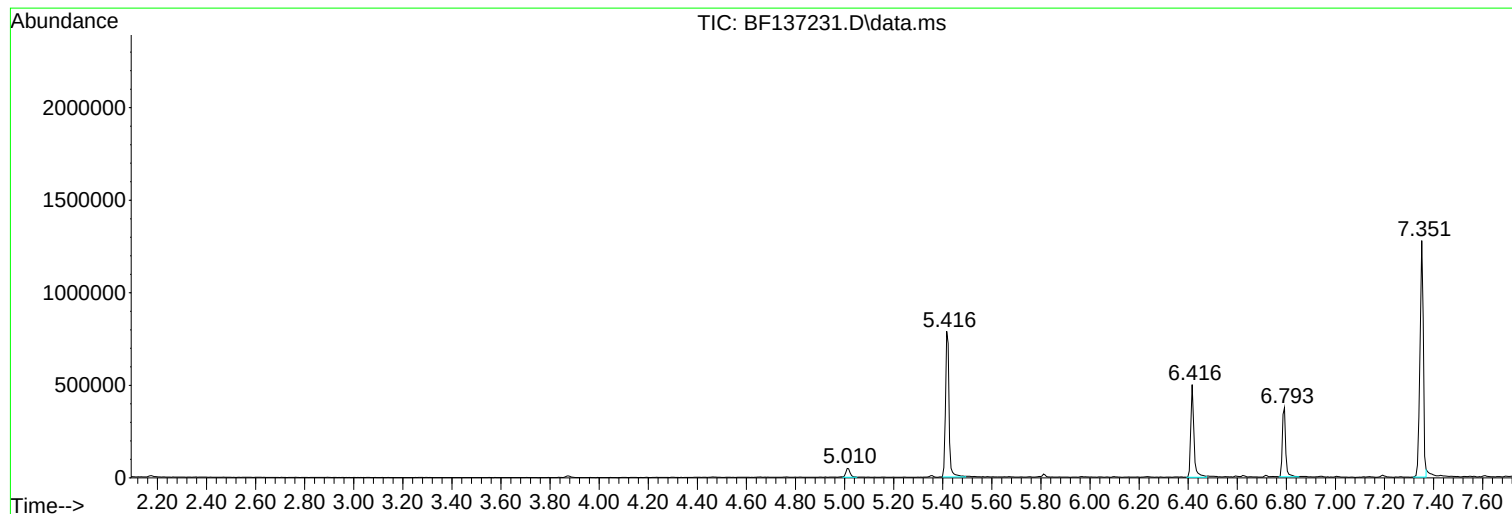
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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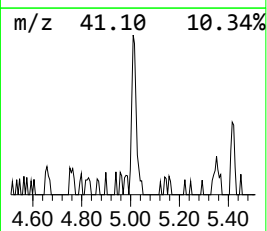
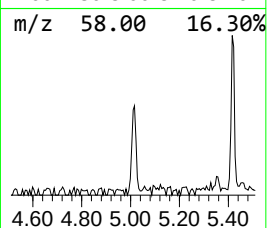
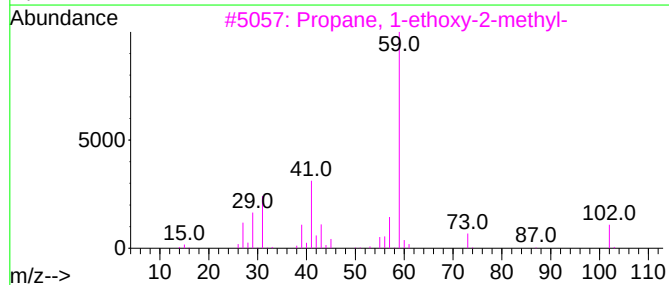
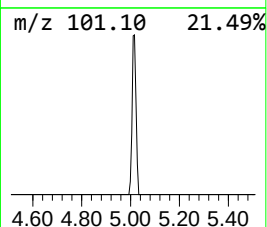
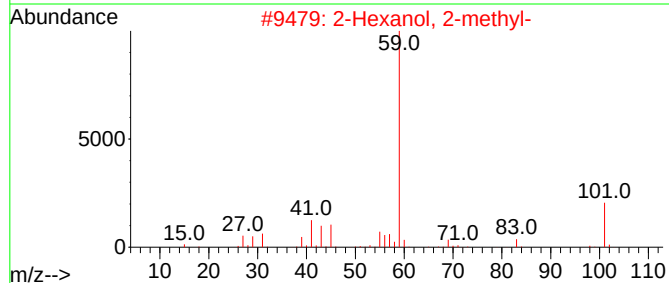
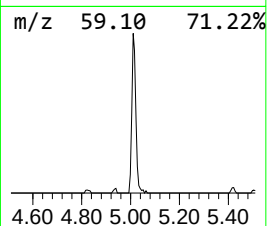
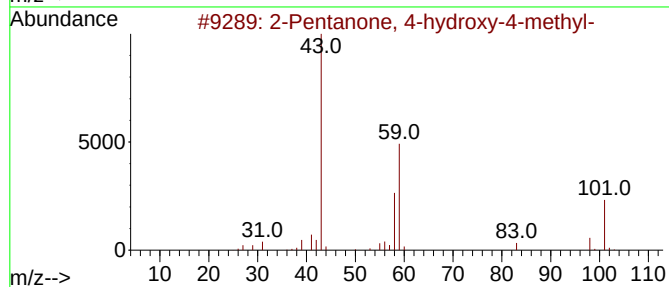
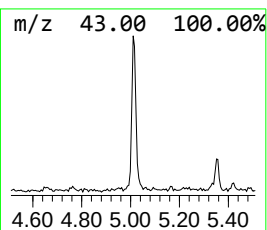
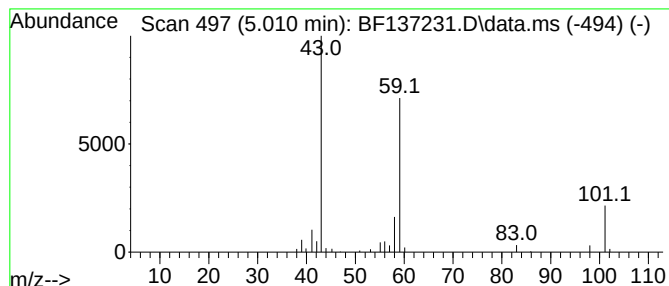
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	3.31 ng	57757	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40		
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38		
4	3-Octanol	130	C8H18O	000589-98-0	36		
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23		



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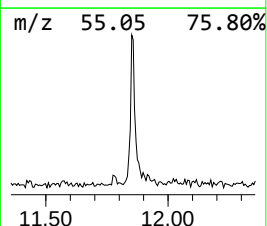
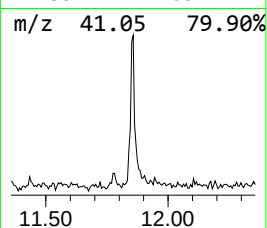
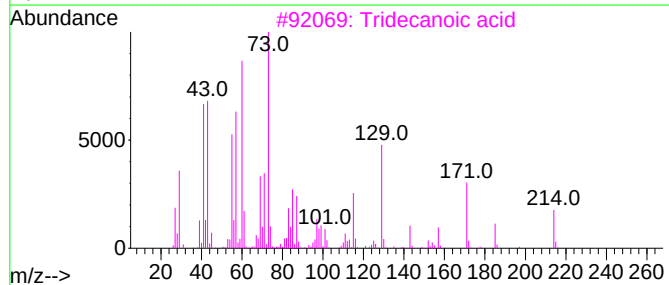
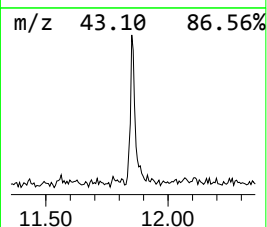
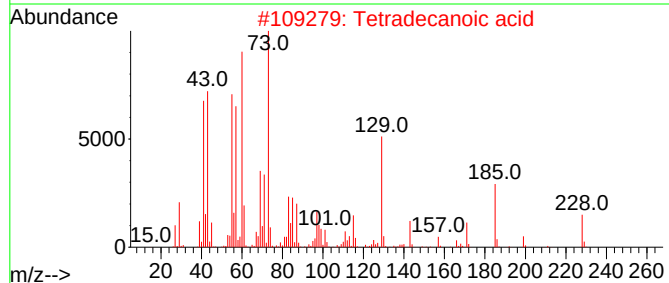
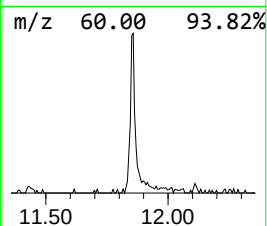
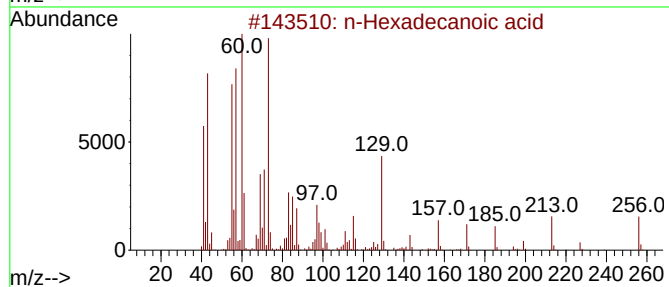
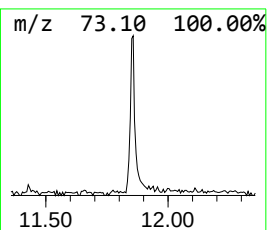
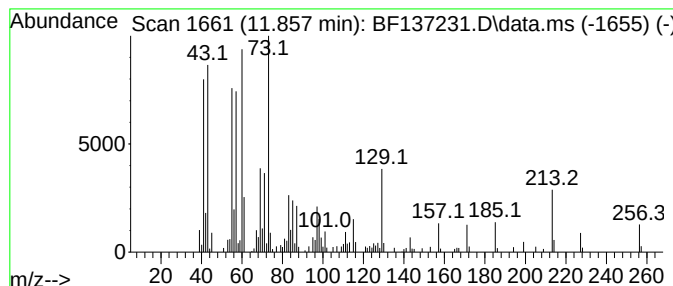
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	7.93 ng	184635	Phenanthrene-d10	11.316

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	94
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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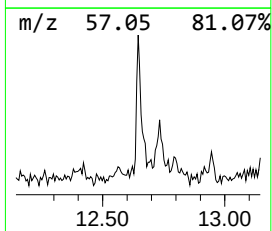
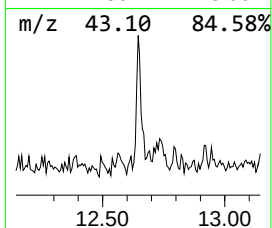
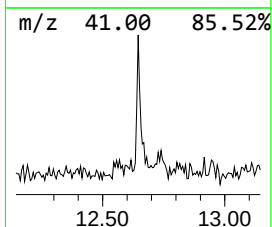
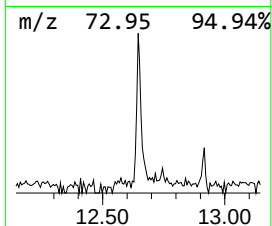
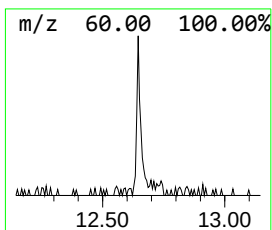
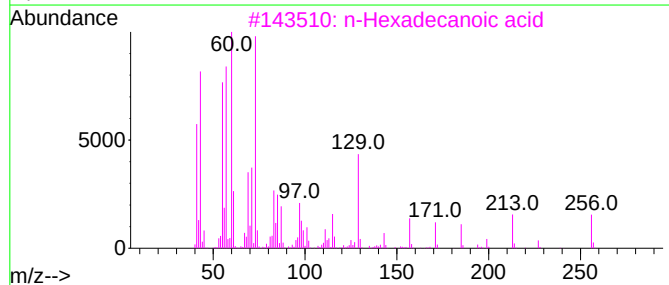
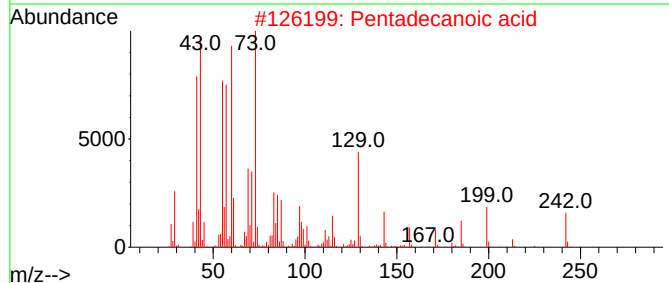
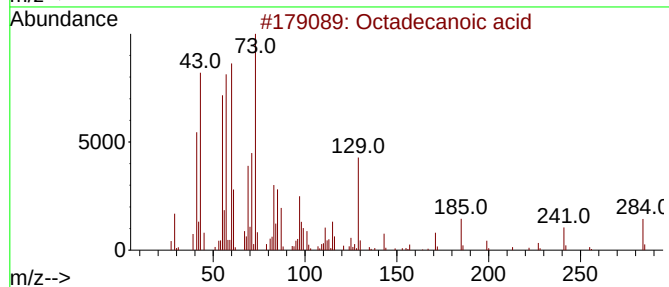
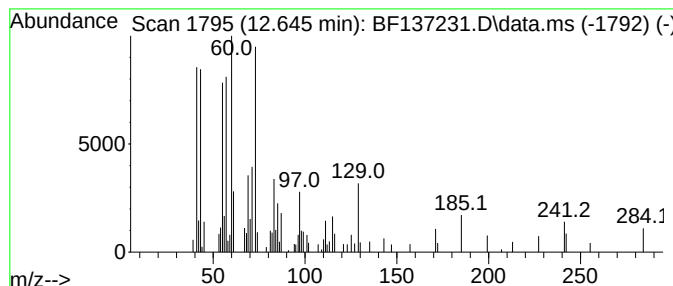
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	3.38 ng	62960	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Propyl tetracosyl ether	396	C27H56O	1000406-28-3	41



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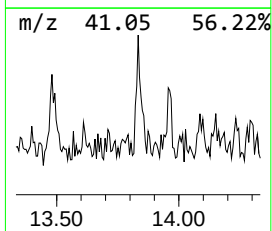
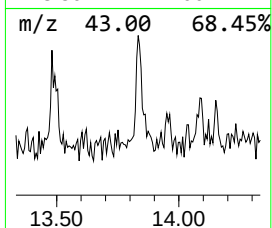
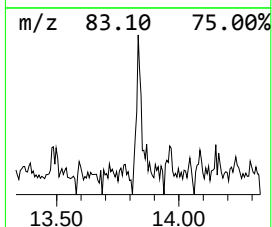
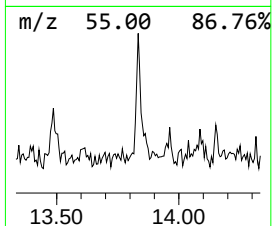
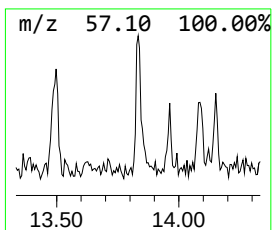
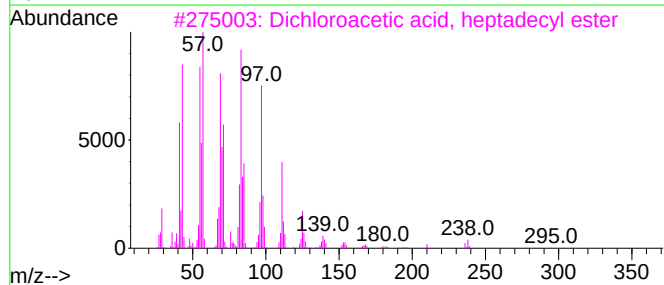
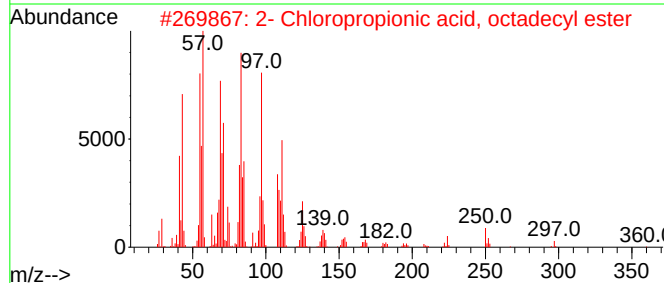
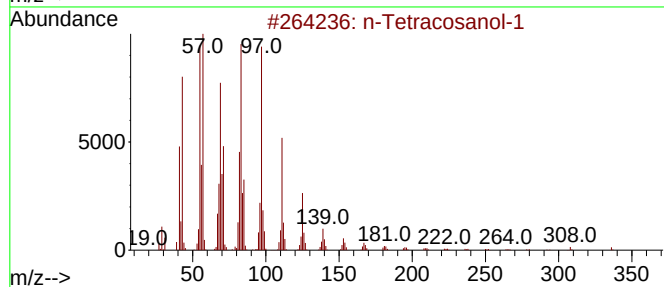
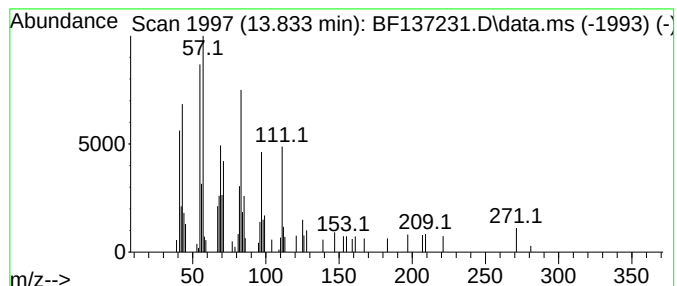
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	2.31 ng	42967	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	81
2			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	81
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	74
4			1-Hexacosanol	382	C26H54O	000506-52-5	74
5			1-Octadecanol	270	C18H38O	000112-92-5	70



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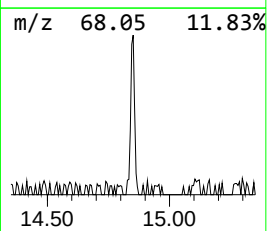
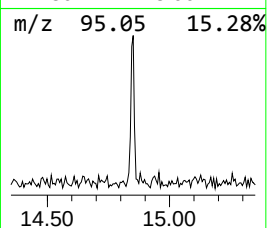
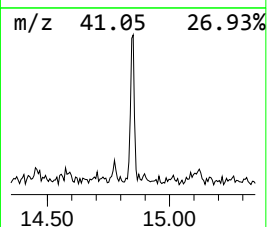
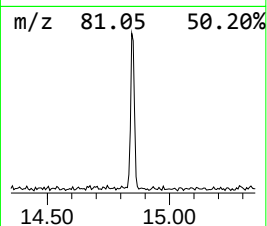
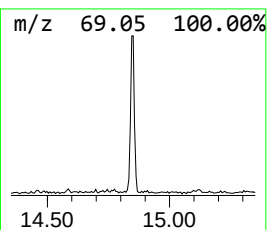
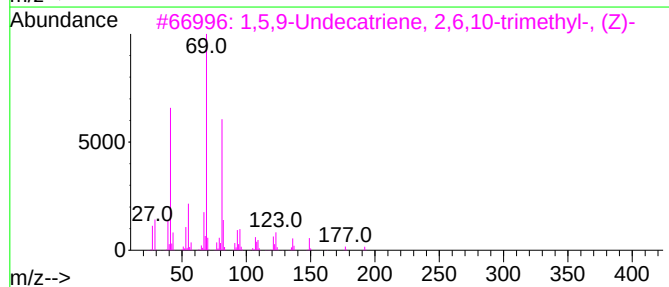
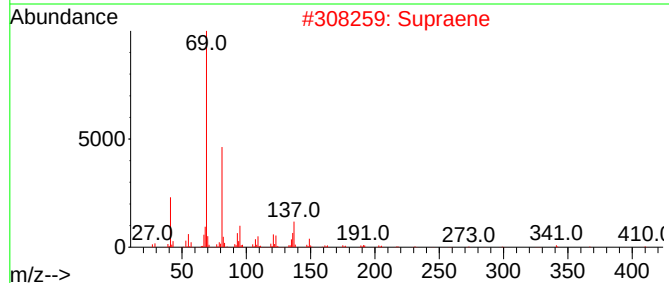
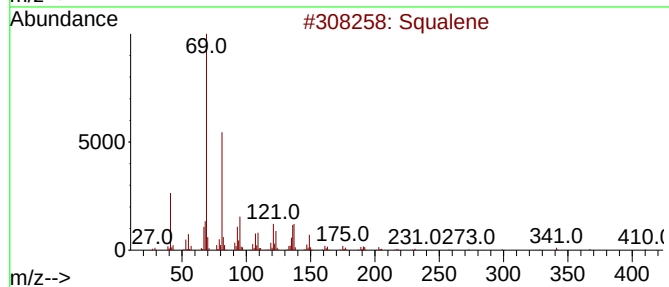
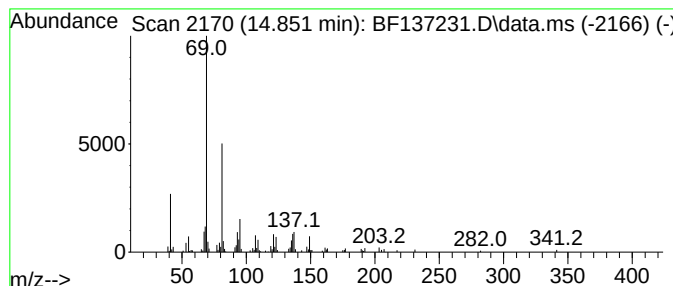
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	5.97 ng	101758	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	83
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.010	3.3	ng	57757	1	6.793	348810	20.0
n-Hexadecanoic ...	11.857	7.9	ng	184635	4	11.316	465448	20.0
Octadecanoic acid	12.645	3.4	ng	62960	5	13.969	372514	20.0
n-Tetracosanol-1	13.833	2.3	ng	42967	5	13.969	372514	20.0
Squalene	14.851	6.0	ng	101758	6	15.451	341119	20.0