

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122922\
 Data File : BF131884.D
 Acq On : 29 Dec 2022 18:23
 Operator : CG\JU
 Sample : N6228-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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_F\Methods\8270-BF122422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131884.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	494	500	514	rVB	601924	809288	41.44%	5.897%
2	5.434	564	569	572	rBV	1908081	1774710	90.88%	12.933%
3	6.451	737	742	745	rBV	1769102	1806006	92.48%	13.161%
4	6.816	800	804	807	rBV	581371	441388	22.60%	3.216%
5	7.387	896	901	904	rBV	1288705	1229561	62.96%	8.960%
6	8.104	1018	1023	1027	rBV	630525	537189	27.51%	3.915%
7	9.186	1202	1207	1210	rBV	2333957	1952894	100.00%	14.231%
8	9.869	1319	1323	1326	rBV	625229	534585	27.37%	3.896%
9	10.657	1453	1457	1461	rBV	1101765	1041677	53.34%	7.591%
10	11.357	1573	1576	1579	rBV	566617	476518	24.40%	3.472%
11	11.380	1579	1580	1584	rVB	77398	50861	2.60%	0.371%
12	11.886	1664	1666	1672	rBV2	72462	61712	3.16%	0.450%
13	12.574	1778	1783	1787	rBV	113142	101530	5.20%	0.740%
14	12.804	1817	1822	1827	rBV	97910	109688	5.62%	0.799%
15	12.951	1843	1847	1850	rBV	1496154	1262088	64.63%	9.197%
16	13.851	1996	2000	2010	rVB2	139318	201585	10.32%	1.469%
17	14.010	2022	2027	2030	rBV	440060	415382	21.27%	3.027%
18	14.033	2030	2031	2034	rVB	39646	28191	1.44%	0.205%
19	14.110	2038	2044	2048	rBV	249821	294289	15.07%	2.145%
20	14.768	2153	2156	2163	rBV	126970	147898	7.57%	1.078%
21	15.057	2202	2205	2208	rBV	31846	47322	2.42%	0.345%
22	15.427	2265	2268	2273	rVB	31044	39490	2.02%	0.288%
23	15.492	2274	2279	2291	rVB	256065	358798	18.37%	2.615%

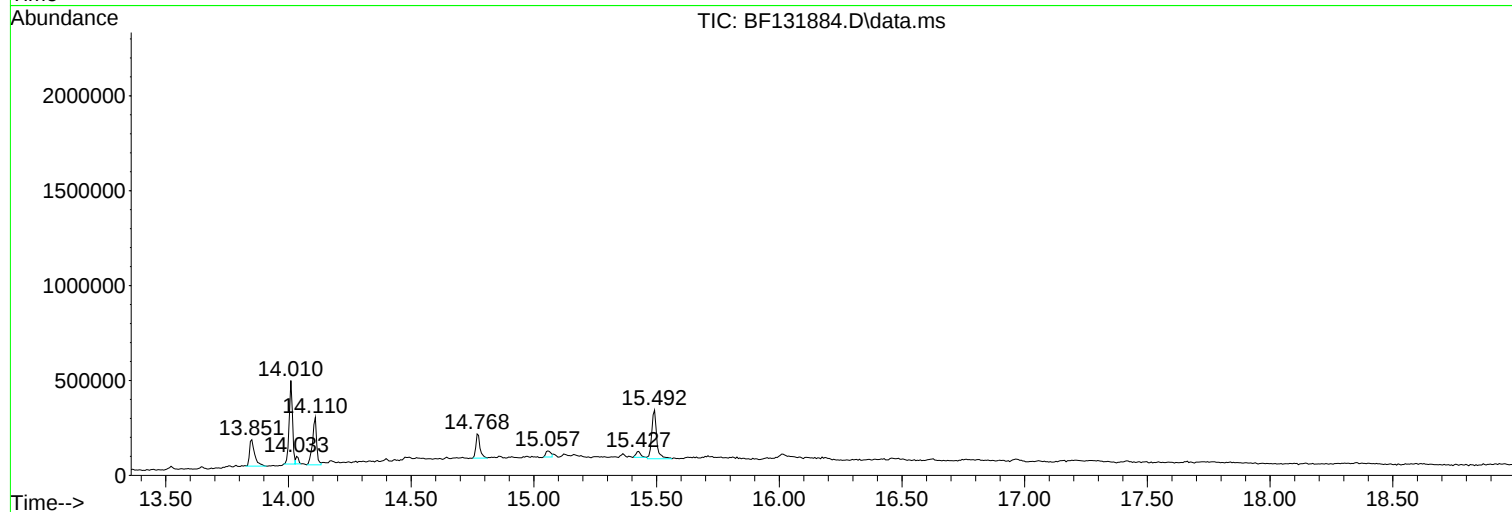
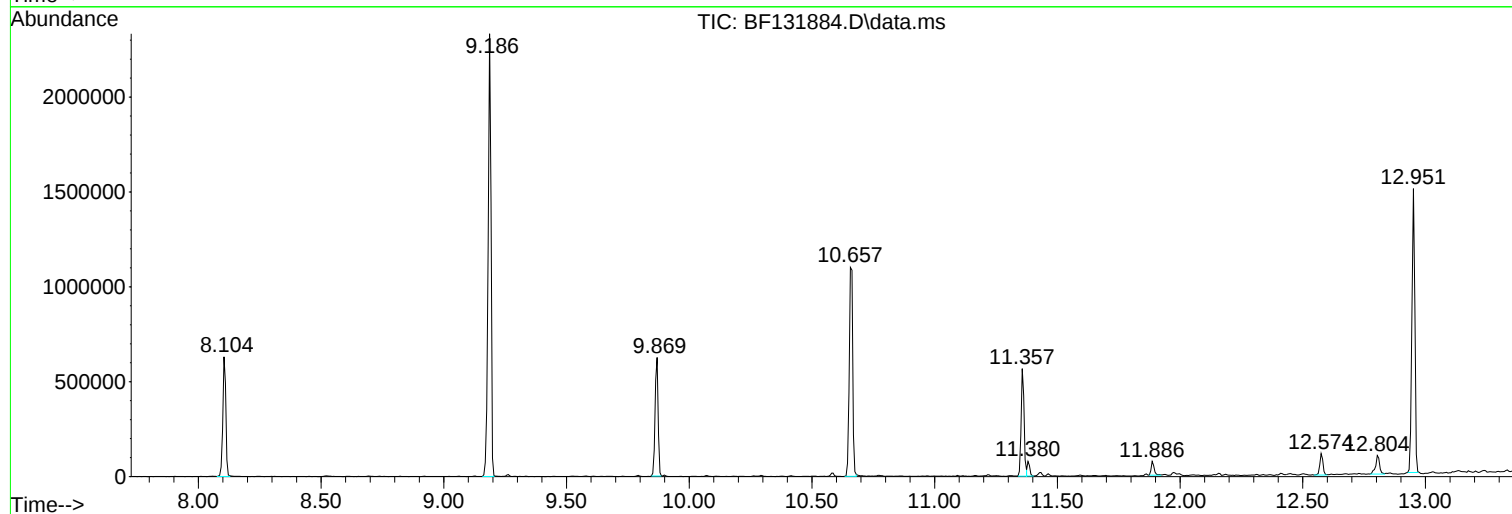
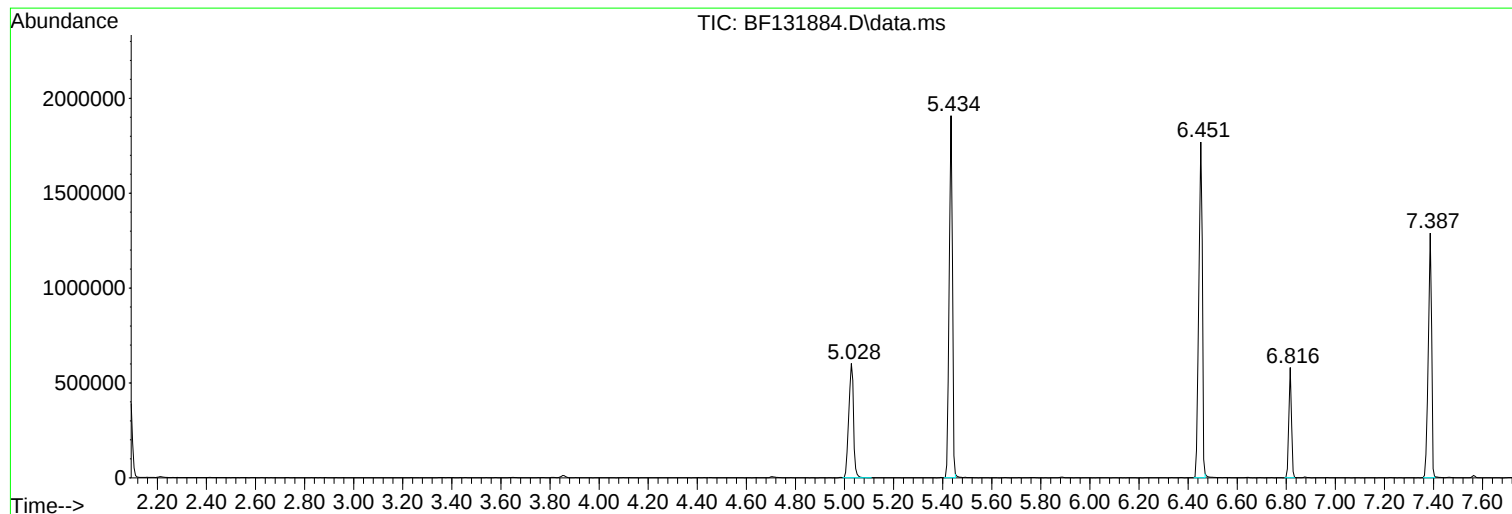
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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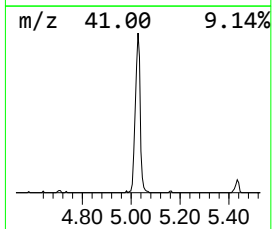
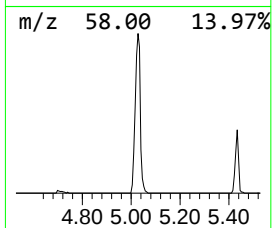
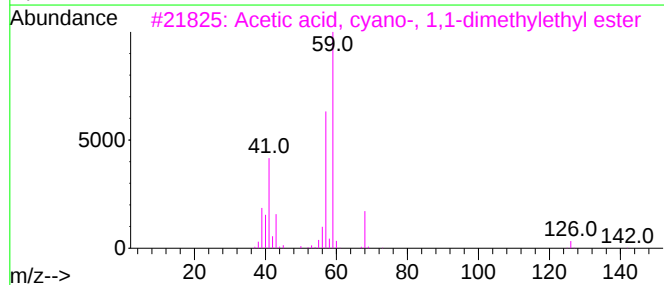
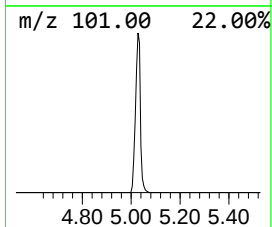
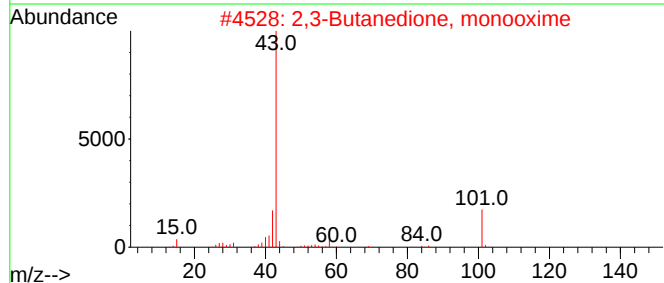
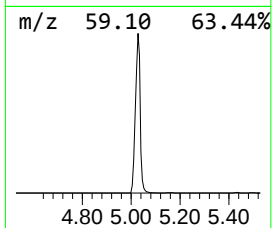
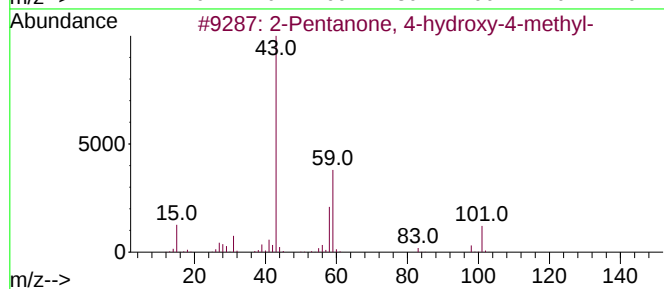
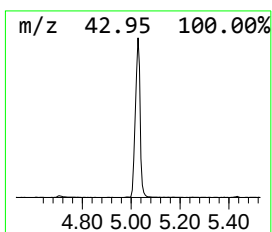
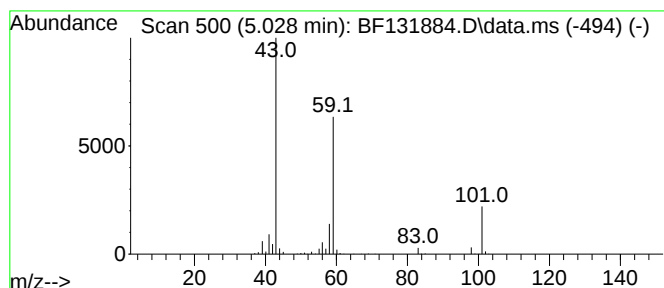
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	36.67 ng	809288	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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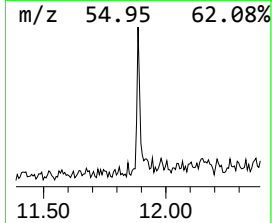
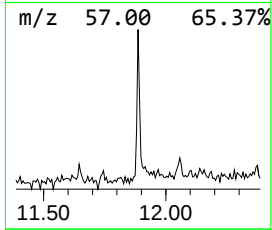
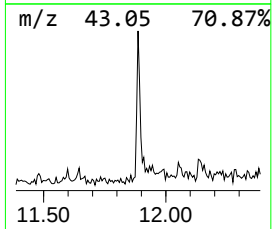
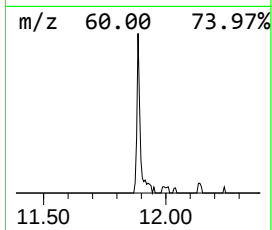
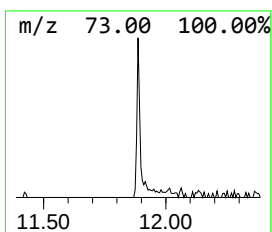
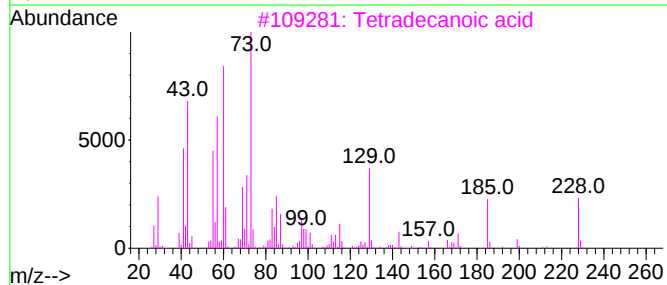
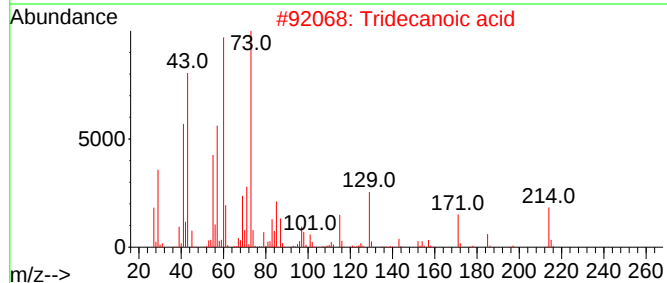
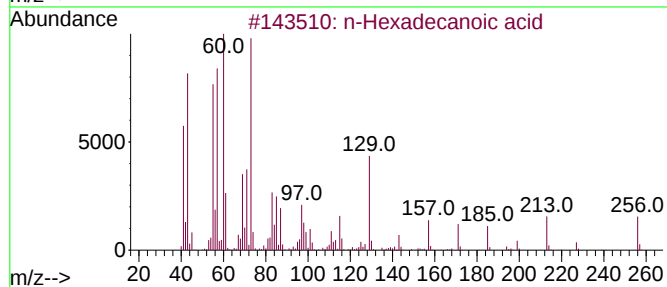
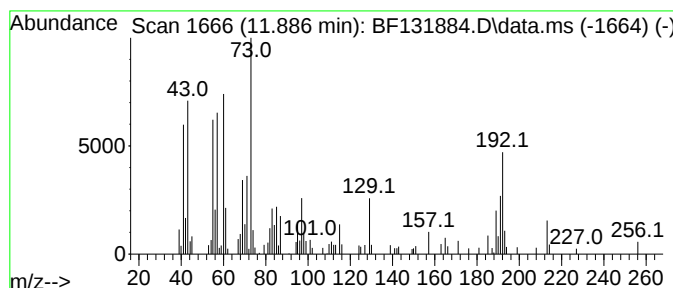
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.59 ng	61712	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Tridecanoic acid	214	C13H26O2	000638-53-9	47
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5			n-Decanoic acid	172	C10H20O2	000334-48-5	38



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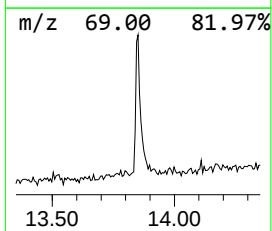
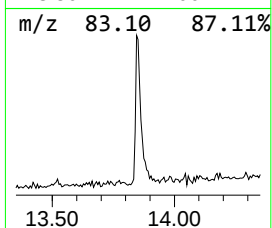
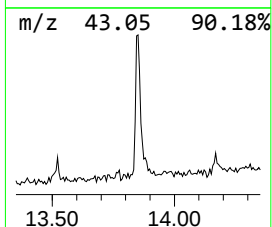
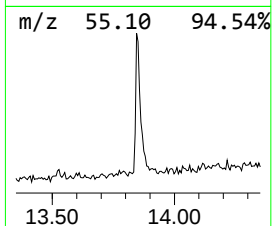
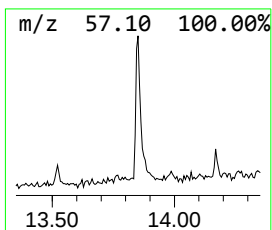
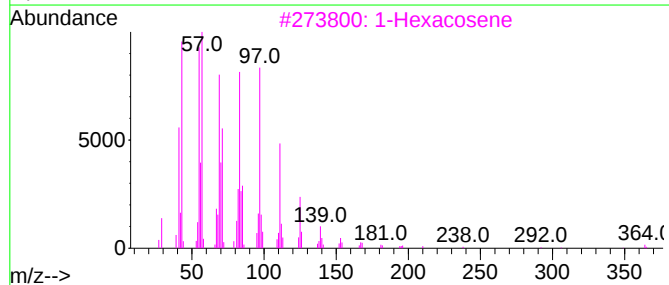
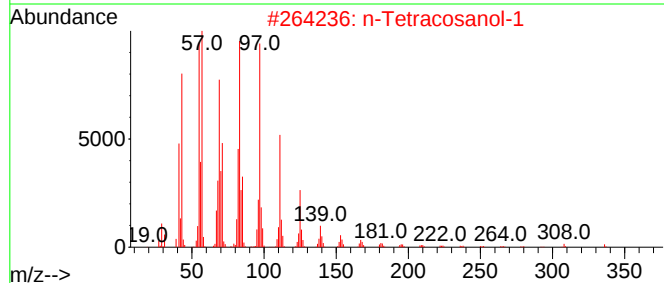
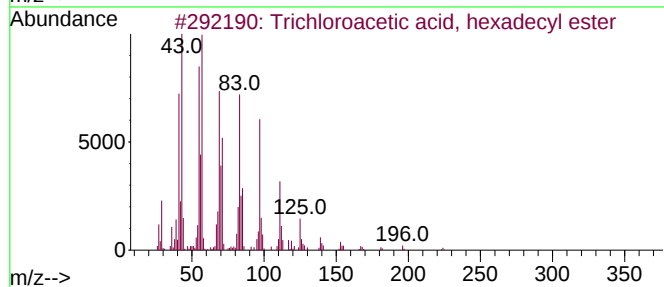
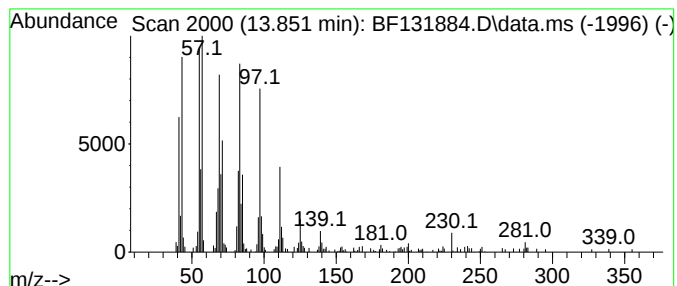
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.851	9.71 ng	201585	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	93



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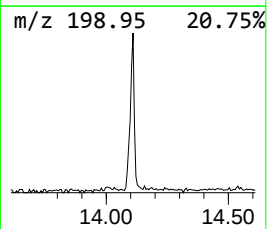
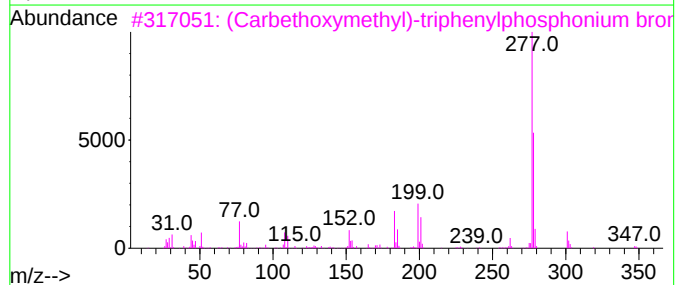
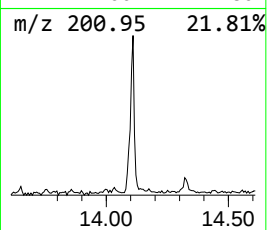
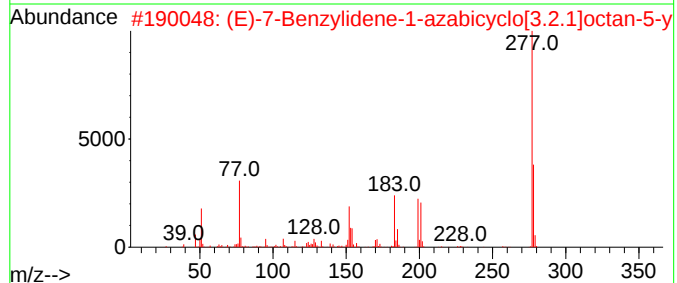
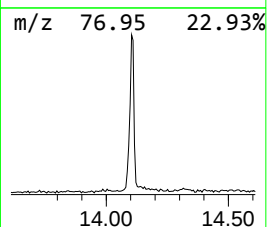
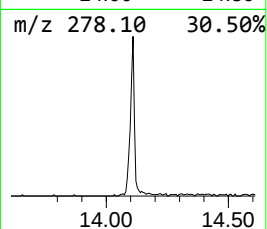
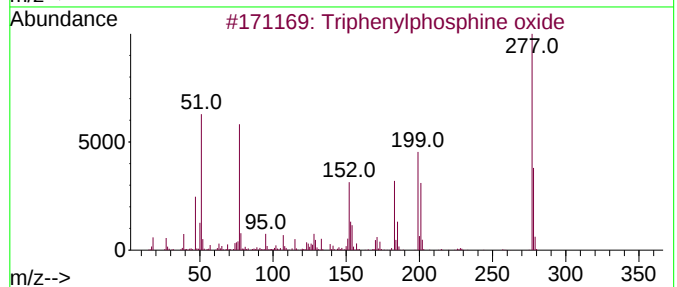
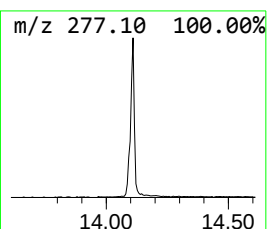
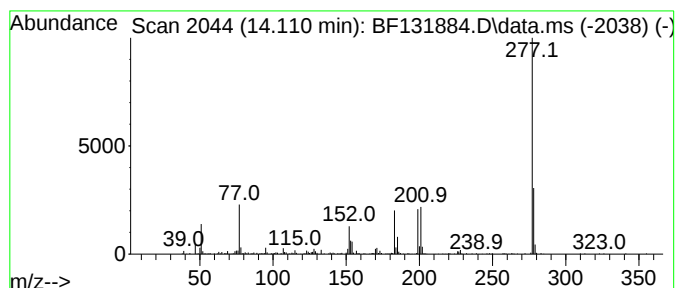
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	14.17 ng	294289	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	70
3			(Carbathoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	38



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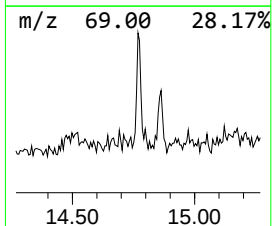
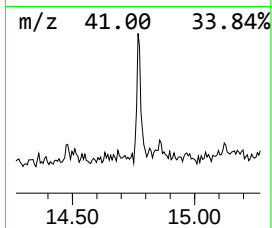
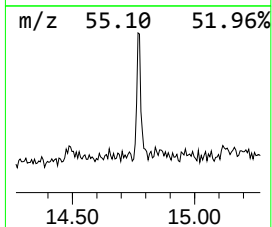
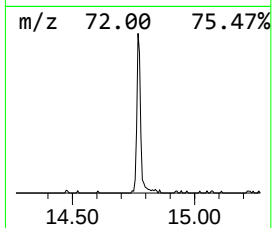
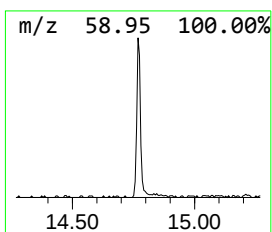
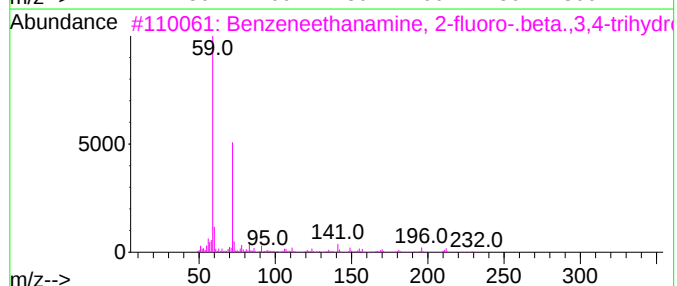
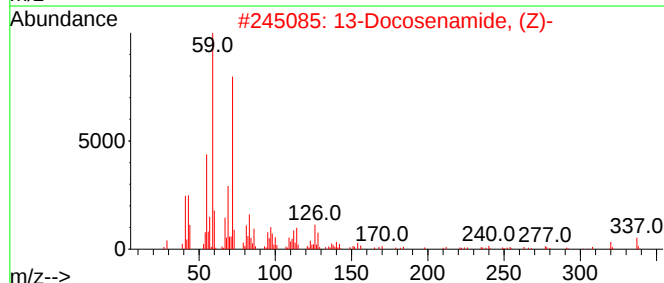
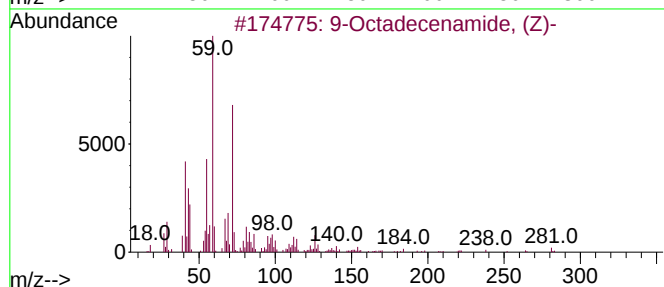
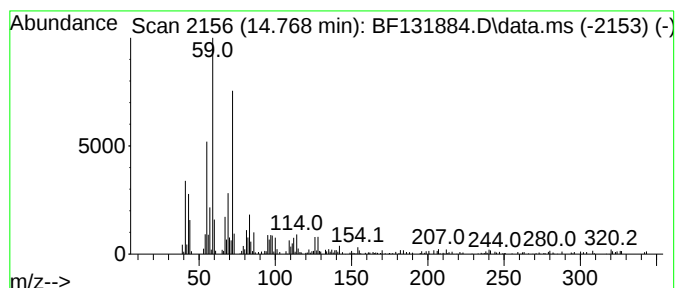
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	8.24 ng	147898	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	72
4			Hexadecanamide	255	C16H33NO	000629-54-9	59
5			Dodecanamide	199	C12H25NO	001120-16-7	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.028	36.7	ng	809288	1	6.816	441388	20.0
n-Hexadecanoic ...	11.886	2.6	ng	61712	4	11.357	476518	20.0
Trichloroacetic...	13.851	9.7	ng	201585	5	14.010	415382	20.0
Triphenylphosph...	14.110	14.2	ng	294289	5	14.010	415382	20.0
9-Octadecenamid...	14.769	8.2	ng	147898	6	15.492	358798	20.0