

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132720.D
Acq On : 09 Mar 2023 16:16
Operator : CG\JU
Sample : 01833-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
42

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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132720.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.216	442	447	461	rVB	1826783	2515264	45.82%	6.654%
2	5.616	510	515	518	rBV	4866624	4656547	84.82%	12.319%
3	6.616	680	685	688	rBV	4341485	4713505	85.86%	12.470%
4	6.981	743	747	750	rBV	1140432	995716	18.14%	2.634%
5	7.545	838	843	846	rBV	3538117	3162705	57.61%	8.367%
6	8.263	961	965	969	rBV	1623117	1279110	23.30%	3.384%
7	9.339	1144	1148	1151	rBV	6291620	5490006	100.00%	14.524%
8	10.022	1261	1264	1268	rBV	1564549	1425270	25.96%	3.771%
9	10.739	1382	1386	1389	rBV	833605	665975	12.13%	1.762%
10	10.822	1395	1400	1403	rBV	3280005	2962032	53.95%	7.836%
11	11.522	1515	1519	1522	rBV	1437573	1255924	22.88%	3.323%
12	13.110	1785	1789	1793	rBV	4810834	4482311	81.64%	11.858%
13	13.580	1864	1869	1875	rBV	1142733	1195031	21.77%	3.162%
14	13.998	1936	1940	1951	rBV	214729	386920	7.05%	1.024%
15	14.180	1967	1971	1974	rBV	1164105	1075234	19.59%	2.845%
16	14.263	1980	1985	1991	rBV	491658	536041	9.76%	1.418%
17	15.721	2228	2233	2240	rVB	791136	1001279	18.24%	2.649%

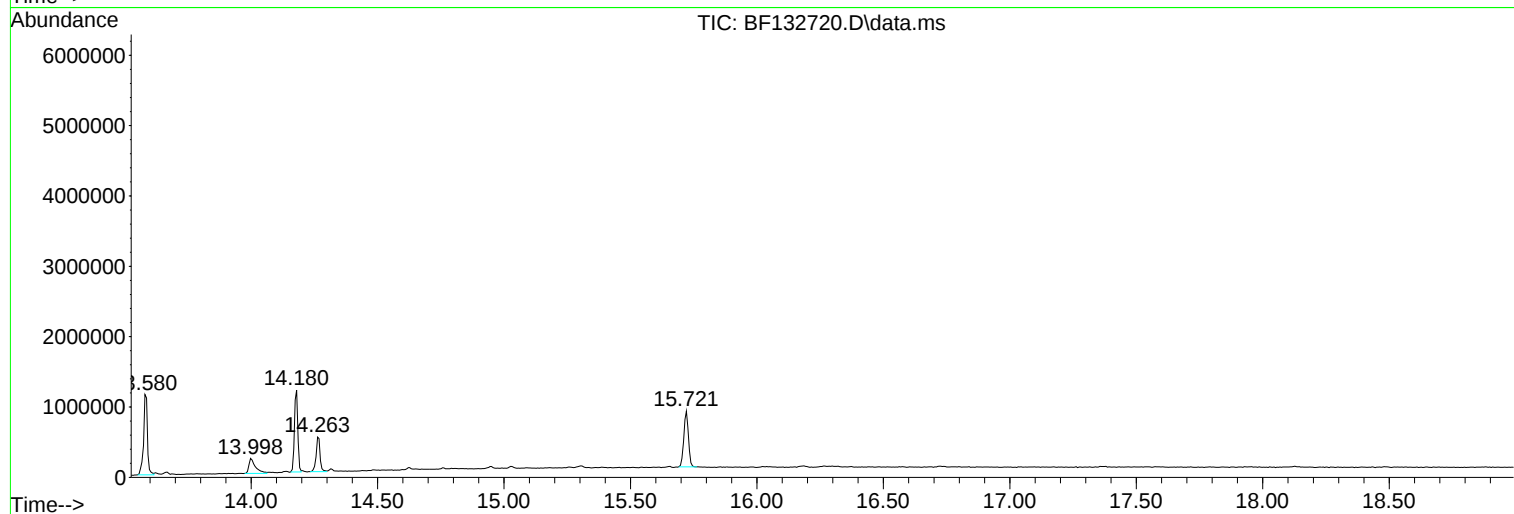
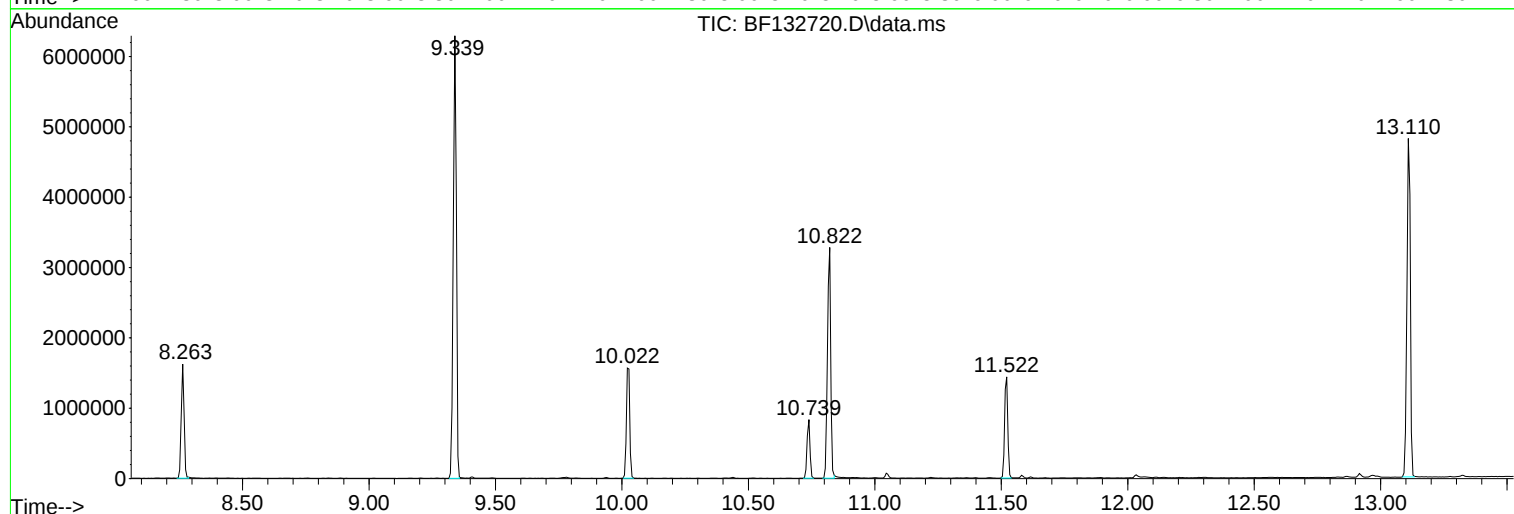
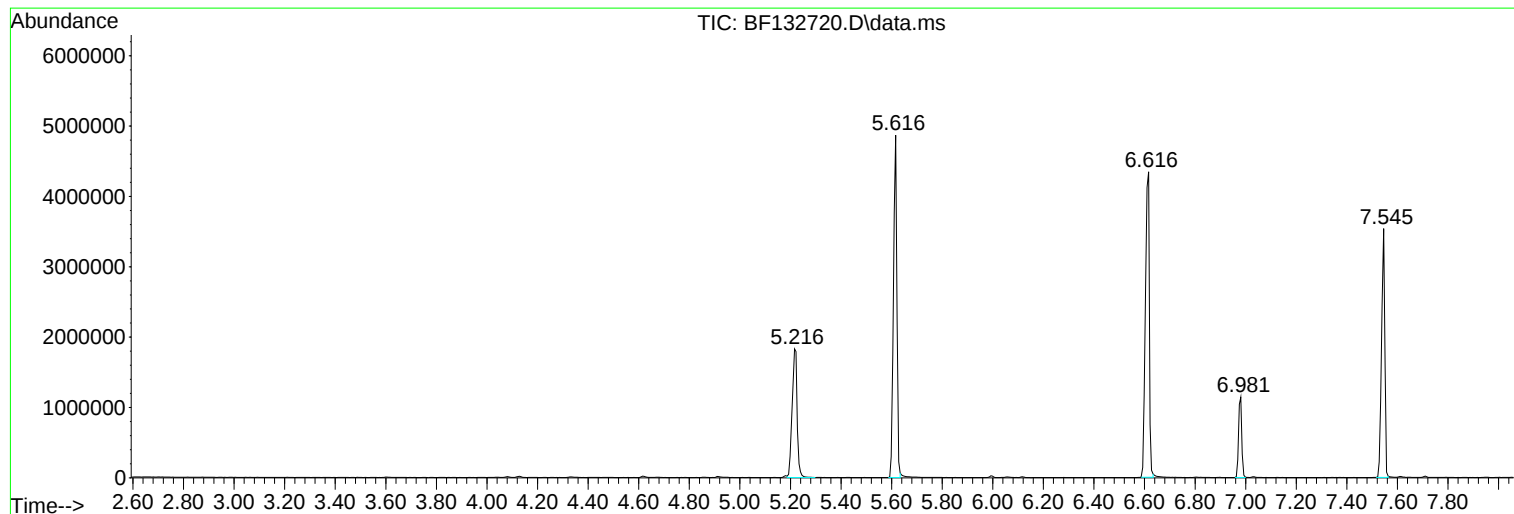
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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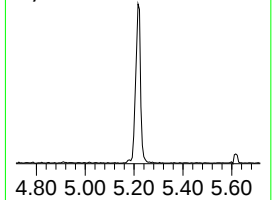
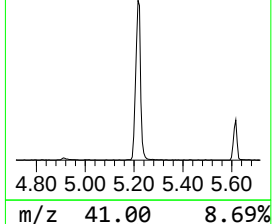
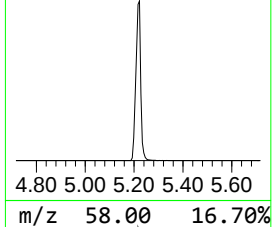
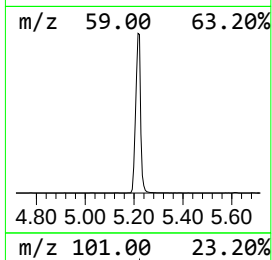
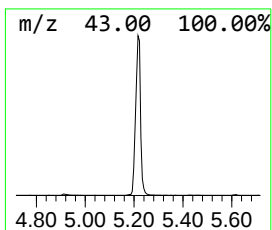
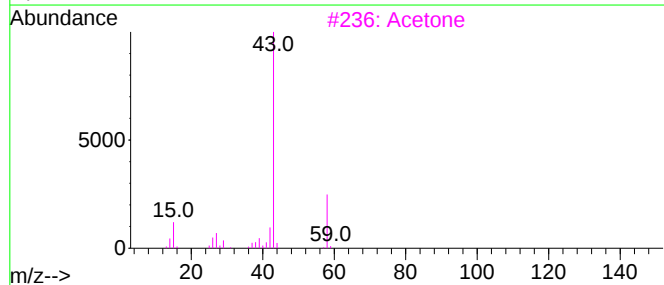
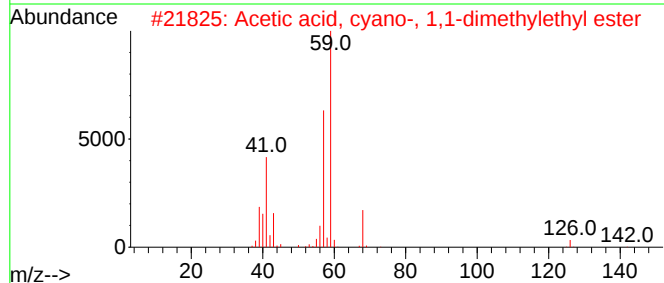
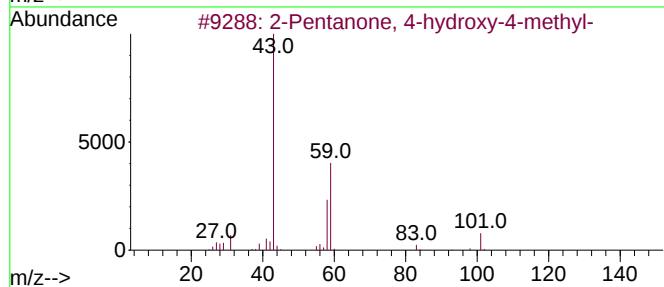
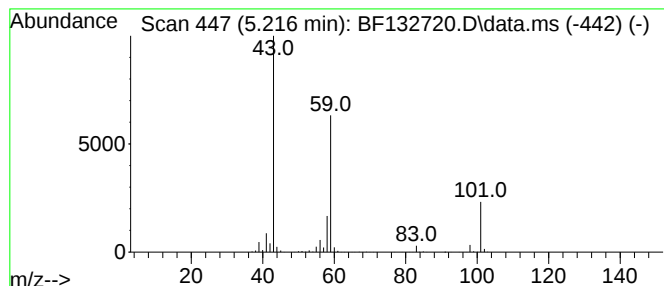
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.216	50.52 ng	2515260	1,4-Dichlorobenzene-d4	6.981

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	17		
3	Acetone	58	C3H6O	000067-64-1	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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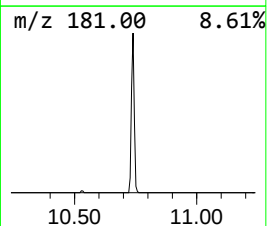
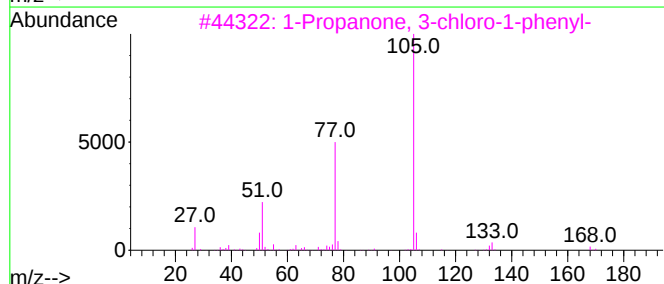
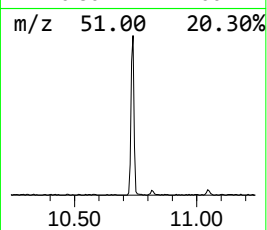
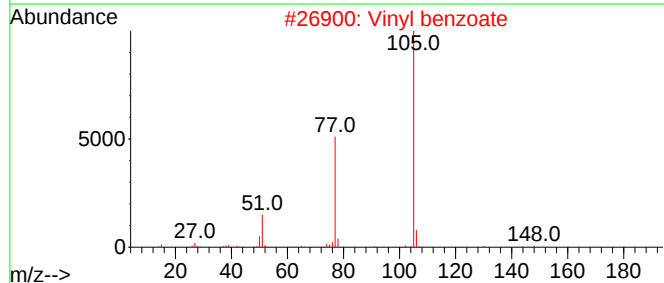
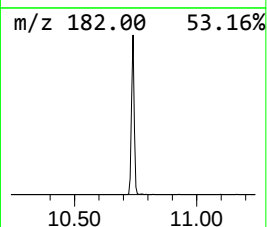
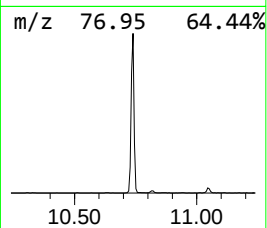
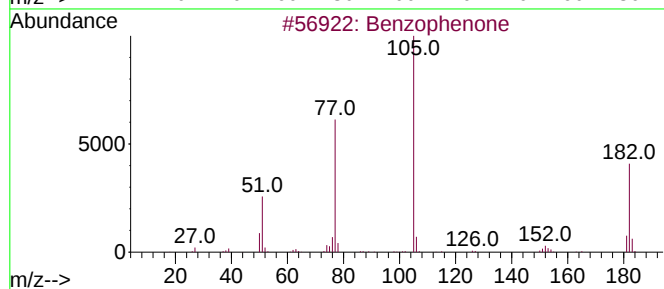
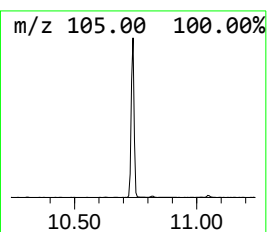
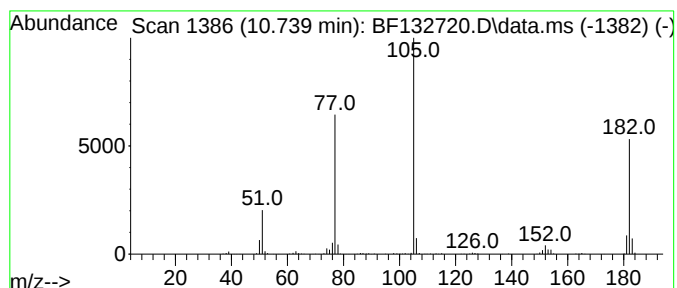
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	9.35 ng	665975	Acenaphthene-d10	10.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Vinyl benzoate	148	C9H8O2	000769-78-8	47
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			Benzofurazan-5-carbohydrazide, N...	282	C14H10N4O3	1000272-94-4	47



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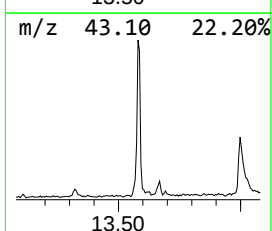
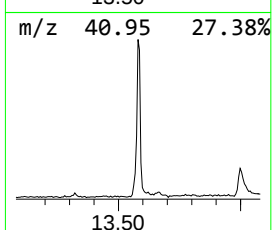
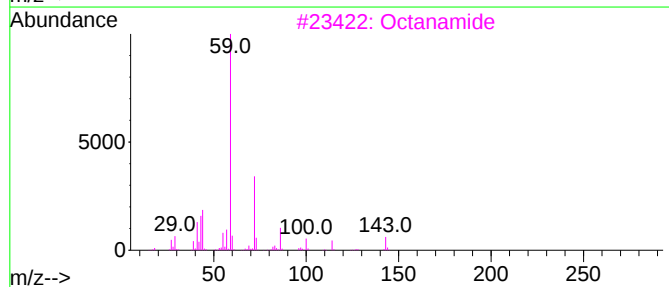
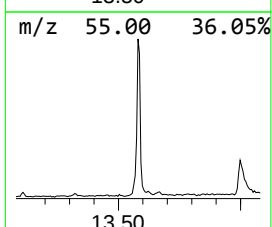
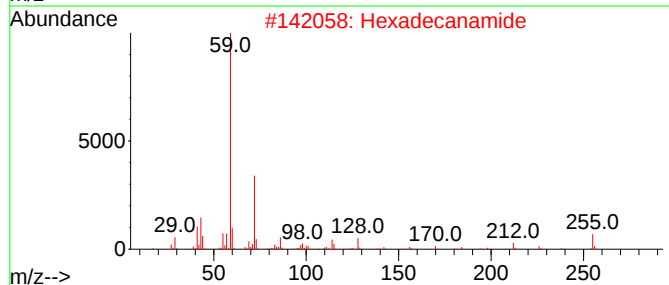
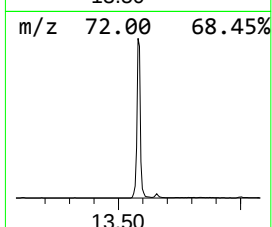
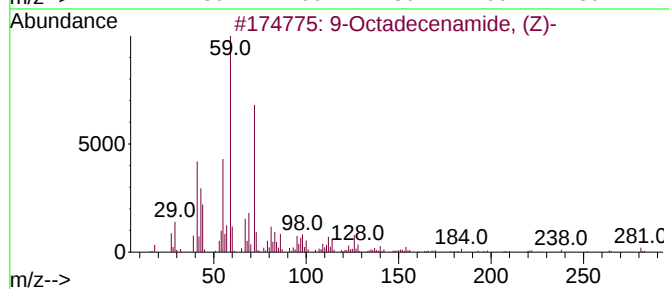
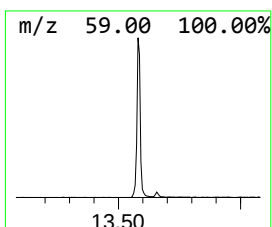
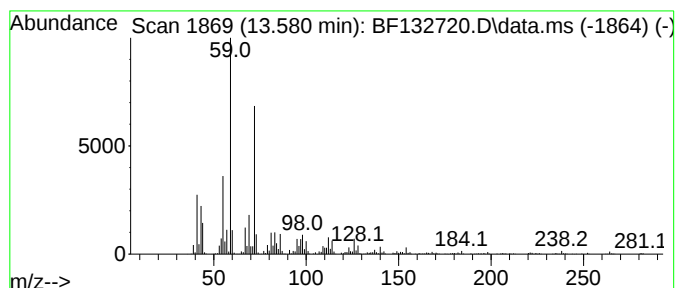
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.580	22.23 ng	1195030	Chrysene-d12	14.180	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	78
3	Octanamide	143	C8H17NO	000629-01-6	64
4	Palmitoleamide	253	C16H31NO	106010-22-4	64
5	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	64



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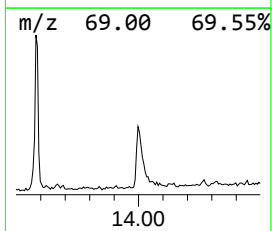
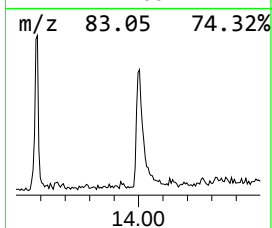
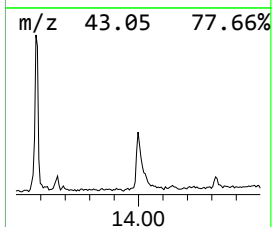
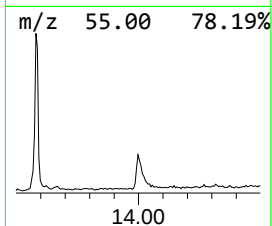
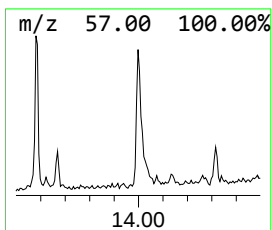
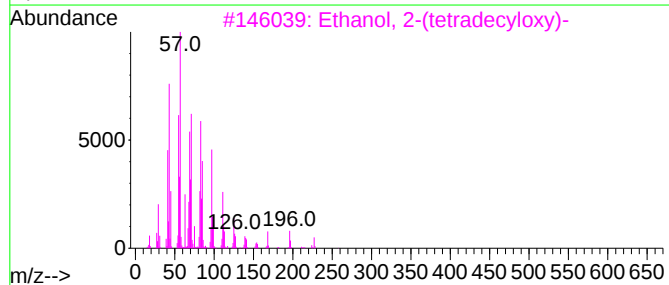
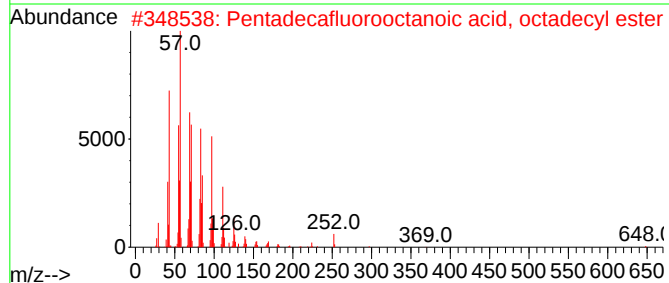
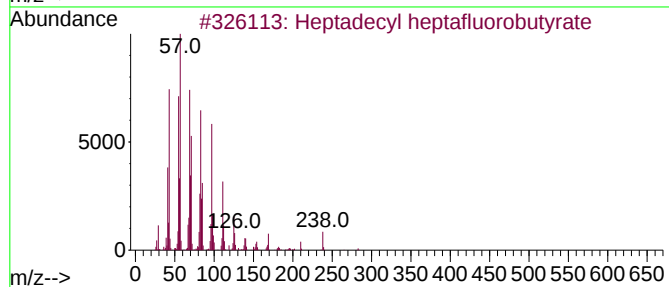
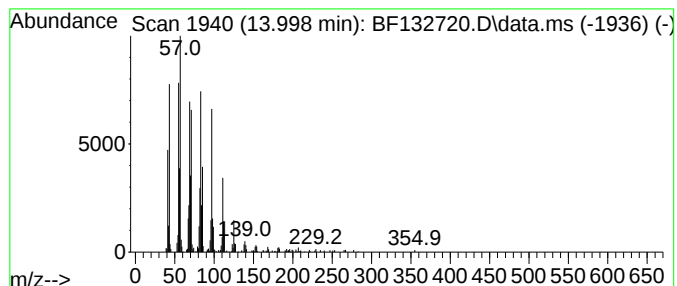
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	7.20 ng	386920	Chrysene-d12	14.180

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5		1-Docosene	308	C22H44	001599-67-3	90



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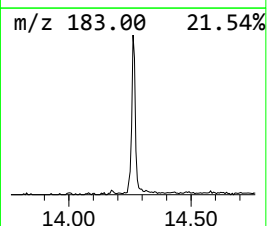
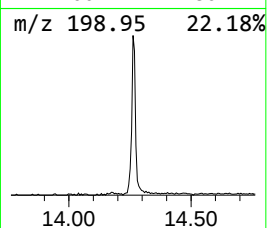
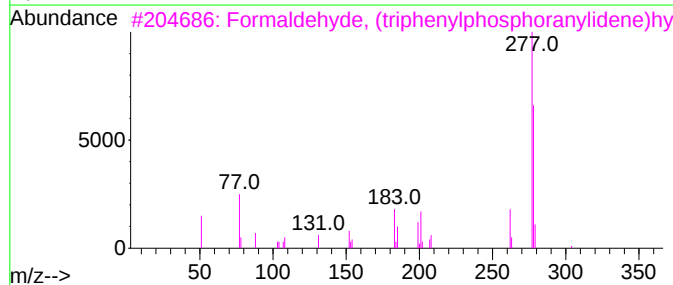
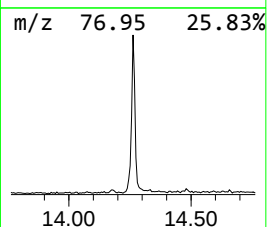
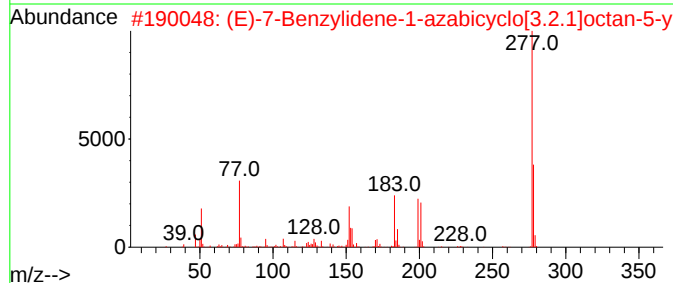
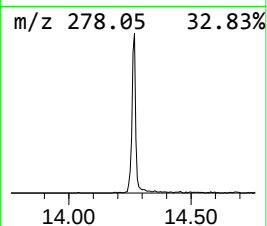
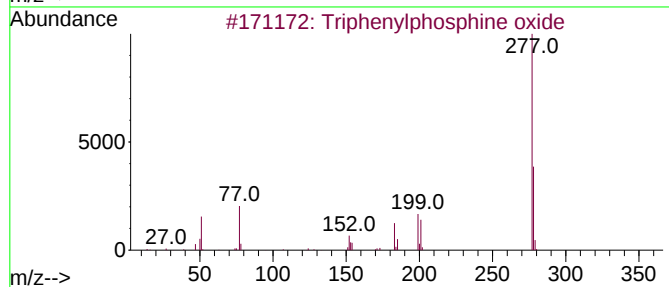
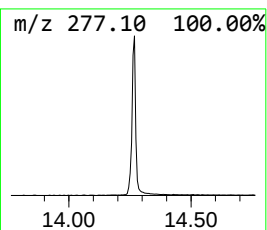
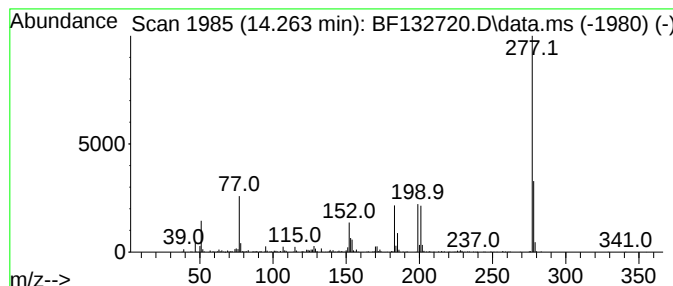
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	9.97 ng	536041	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	70
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	46
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.216	50.5	ng	2515260	1	6.981	995716	20.0
Benzophenone	10.739	9.3	ng	665975	3	10.022	1425270	20.0
9-Octadecenamid...	13.580	22.2	ng	1195030	5	14.180	1075230	20.0
Heptadecyl hept...	13.998	7.2	ng	386920	5	14.180	1075230	20.0
Triphenylphosph...	14.262	10.0	ng	536041	5	14.180	1075230	20.0