

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042023\
 Data File : BF132939.D
 Acq On : 20 Apr 2023 15:16
 Operator : CG\JU
 Sample : 02270-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-17-14-16-20230410

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-BF041723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132939.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	483	488	498	rVB	460033	571317	8.12%	1.135%
2	5.369	552	558	561	rBV	6348109	6523669	92.68%	12.963%
3	6.387	726	731	734	rBV	6115972	6699215	95.17%	13.312%
4	6.757	791	794	797	rBV	2511327	1896673	26.95%	3.769%
5	6.822	802	805	812	rBV	237940	178980	2.54%	0.356%
6	7.322	885	890	893	rBV	4980395	4224774	60.02%	8.395%
7	8.040	1009	1012	1016	rBV	2892348	2504347	35.58%	4.976%
8	9.122	1192	1196	1199	rVB	8785402	7039029	100.00%	13.988%
9	9.398	1236	1243	1251	rBV	213348	181846	2.58%	0.361%
10	9.798	1307	1311	1314	rBV	3165958	2610028	37.08%	5.186%
11	10.510	1428	1432	1435	rBV	437530	375980	5.34%	0.747%
12	10.581	1440	1444	1448	rBV	4355087	3953686	56.17%	7.857%
13	11.281	1559	1563	1566	rBV	2616716	2336309	33.19%	4.643%
14	11.816	1647	1654	1669	rBV2	481071	546334	7.76%	1.086%
15	12.598	1783	1787	1798	rBV	124102	154365	2.19%	0.307%
16	12.869	1828	1833	1836	rBV	6749514	5896067	83.76%	11.716%
17	13.774	1983	1987	1999	rBV2	280801	575338	8.17%	1.143%
18	13.916	2007	2011	2014	rBV	1835539	1682075	23.90%	3.343%
19	14.010	2022	2027	2038	rBV	527917	618632	8.79%	1.229%
20	14.251	2065	2068	2072	rBV	123221	124742	1.77%	0.248%
21	14.404	2091	2094	2100	rBV	64291	91919	1.31%	0.183%
22	15.345	2249	2254	2258	rBV	1329854	1538324	21.85%	3.057%

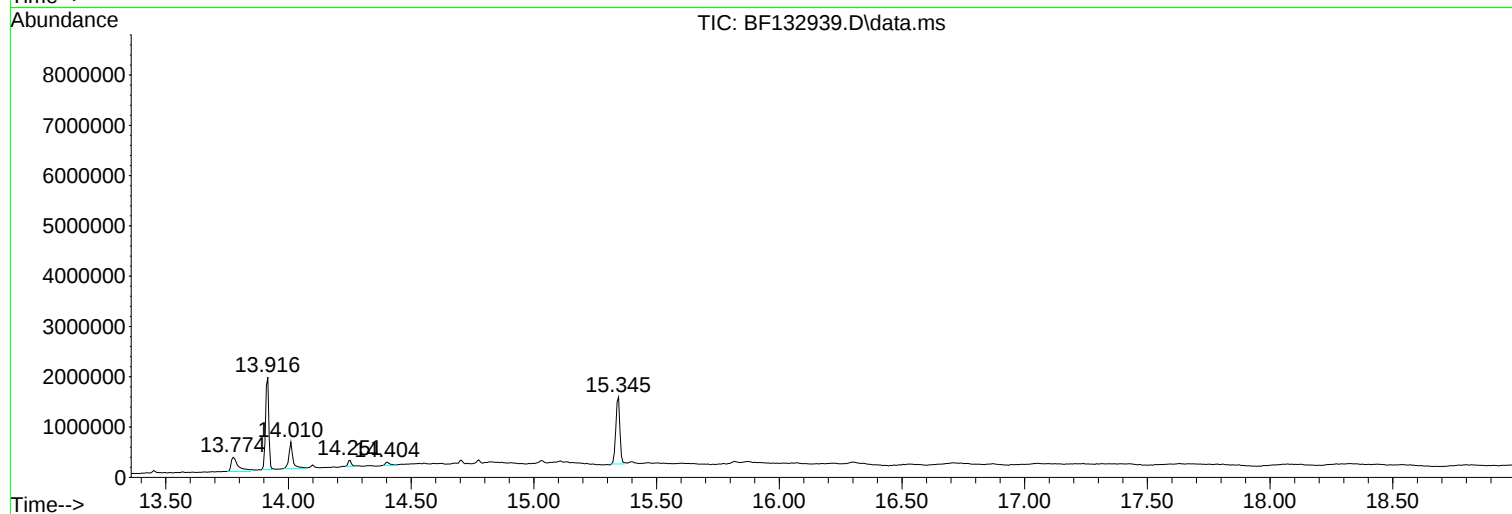
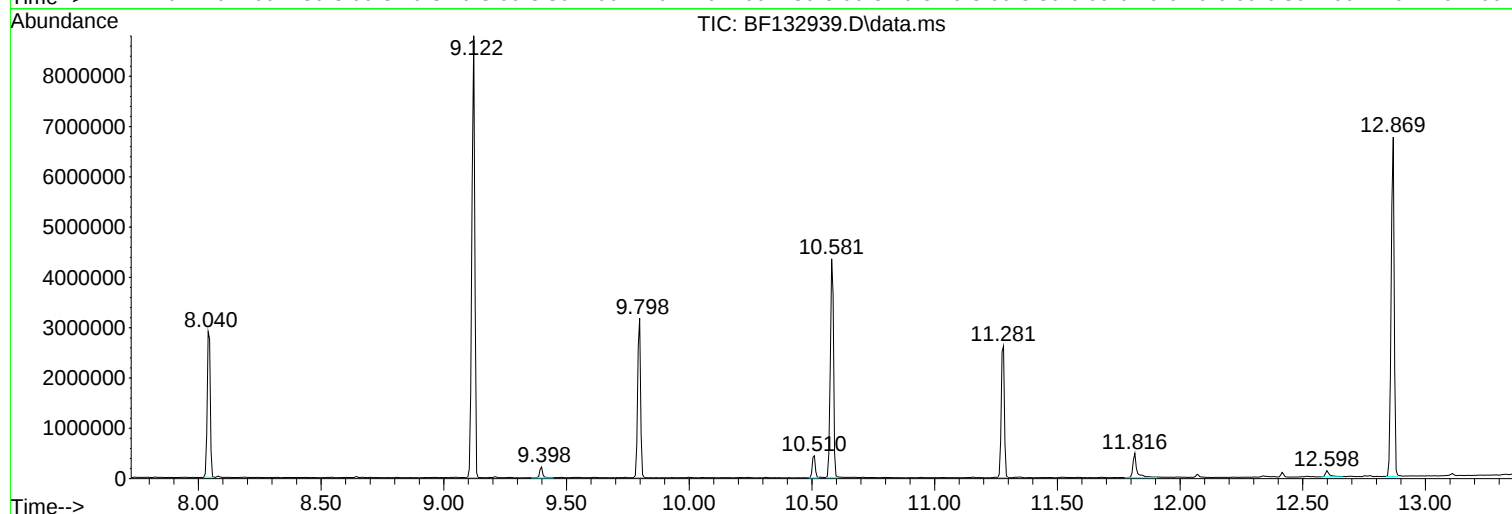
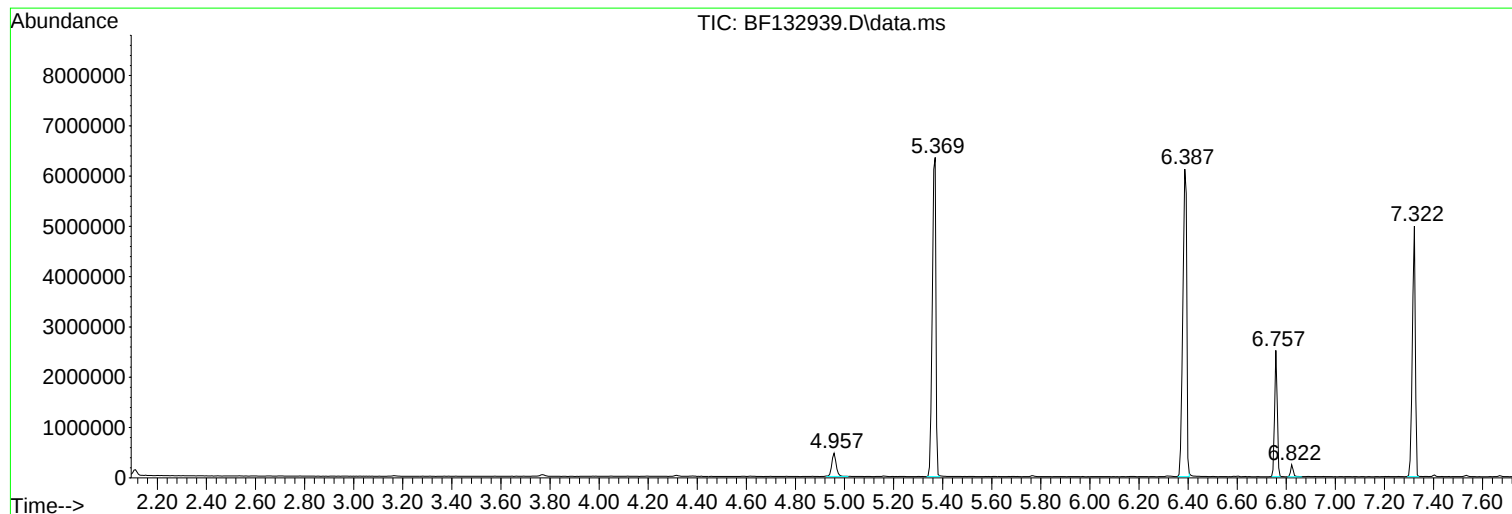
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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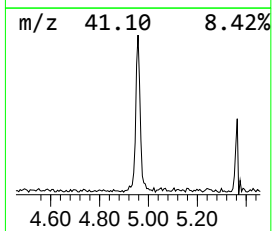
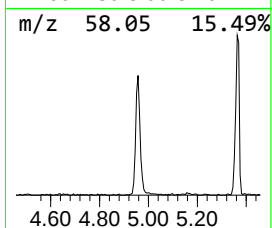
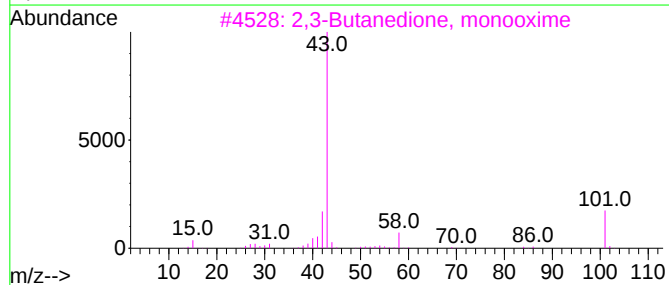
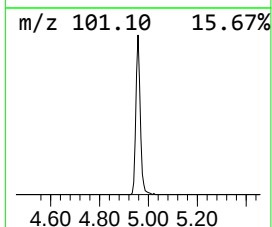
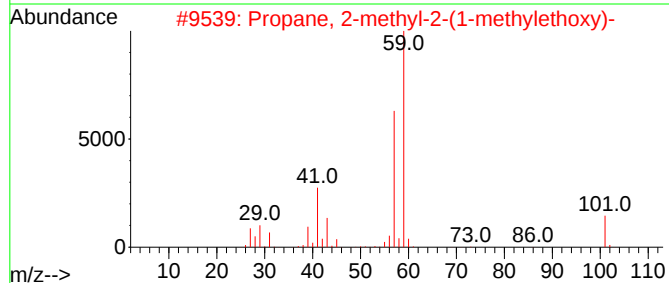
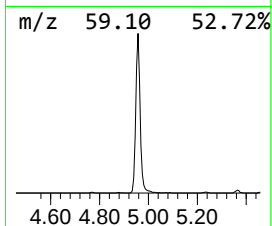
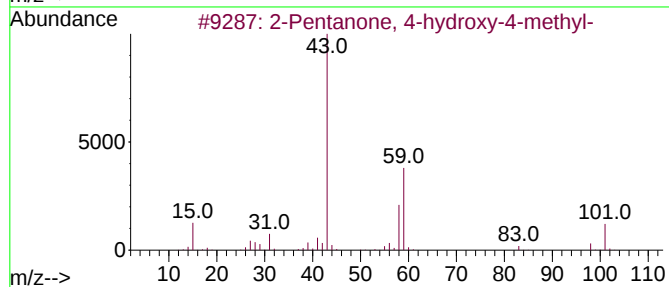
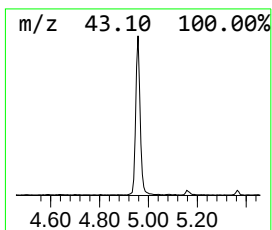
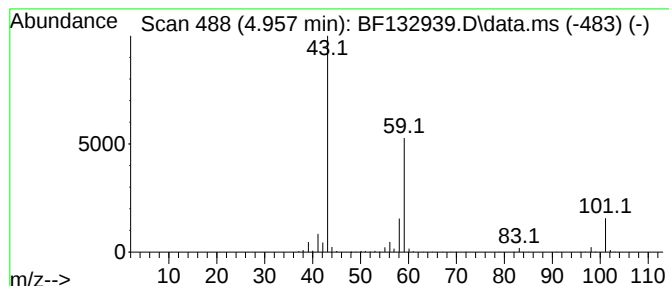
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	6.02 ng	571317	1,4-Dichlorobenzene-d4	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		Allyl acetate	100	C5H8O2	000591-87-7	9



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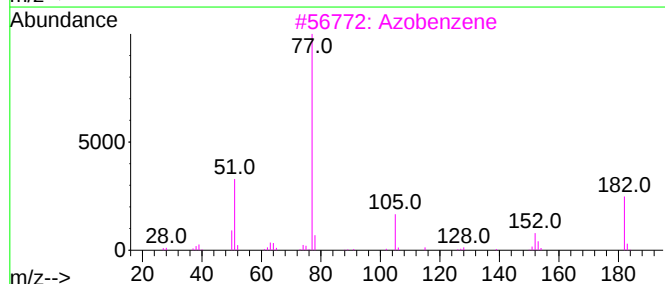
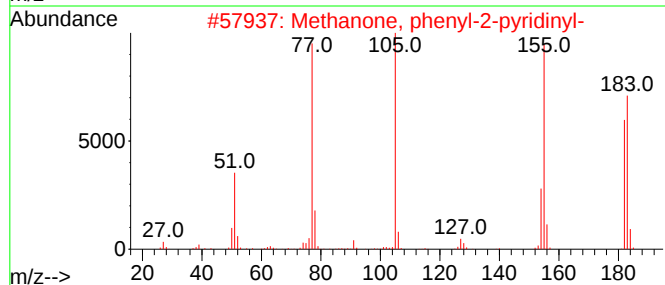
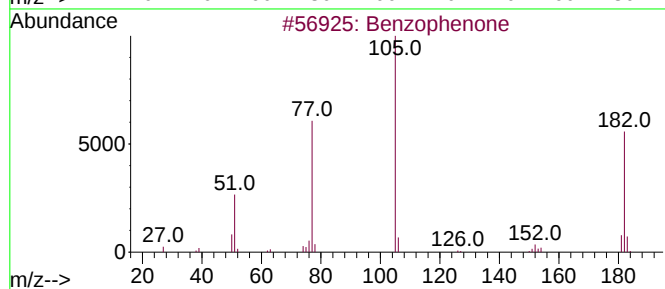
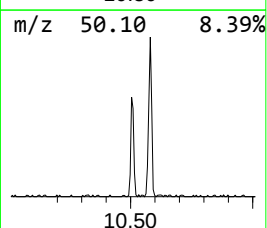
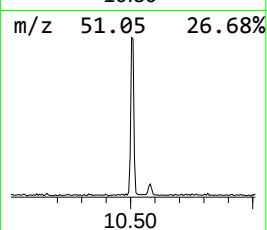
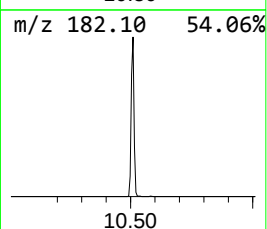
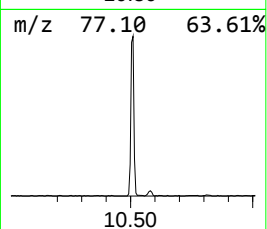
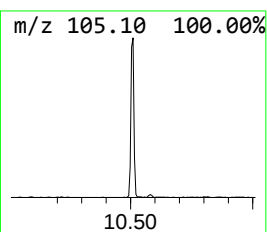
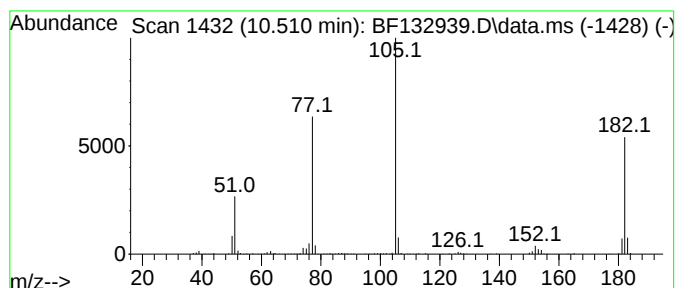
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.510	2.88 ng	375980	Acenaphthene-d10	9.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72
3			Azobenzene	182	C12H10N2	000103-33-3	59
4			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49



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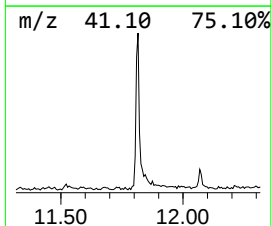
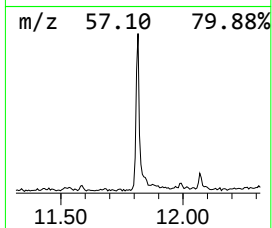
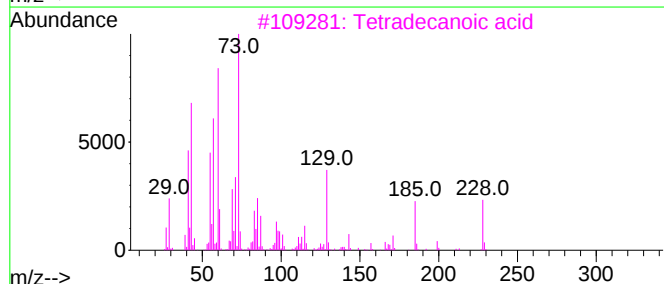
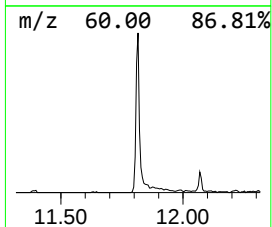
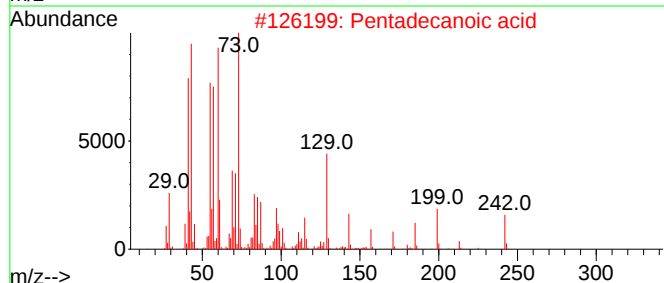
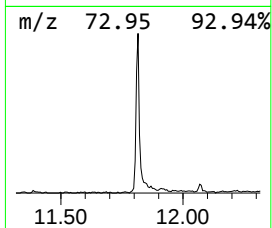
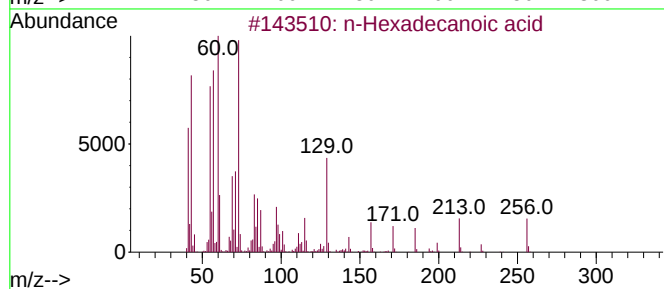
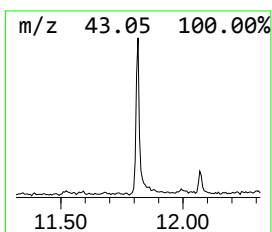
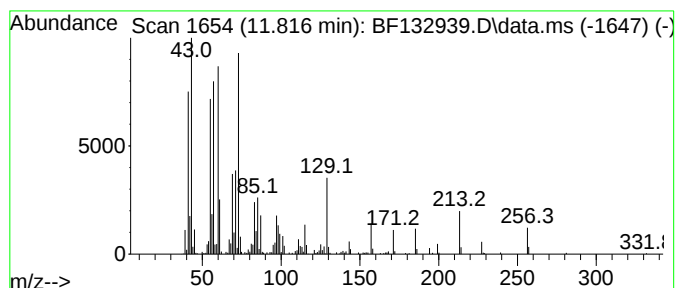
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	4.68 ng	546334	Phenanthrene-d10	11.281

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	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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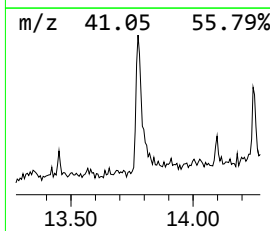
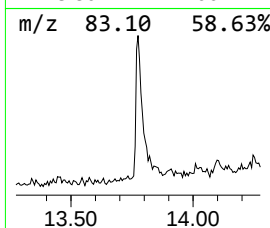
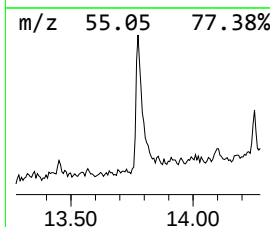
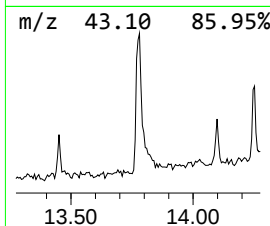
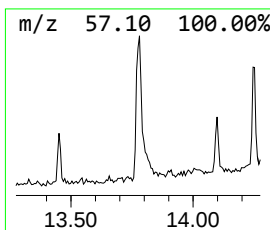
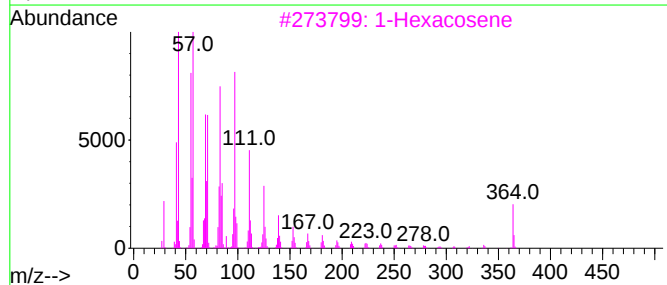
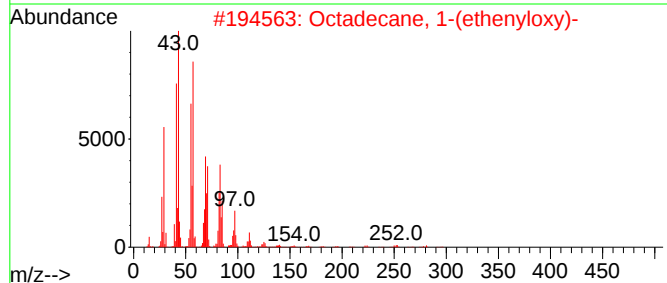
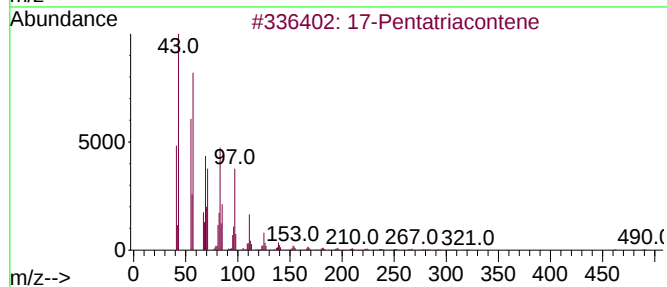
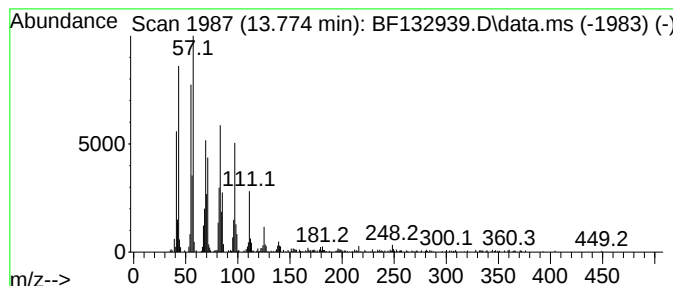
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Peak Number 4 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.775	6.84 ng	575338	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	94
2			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	93
3			1-Hexacosene	364	C26H52	018835-33-1	93
4			9-Hexacosene	364	C26H52	071502-22-2	93
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



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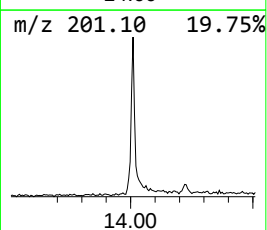
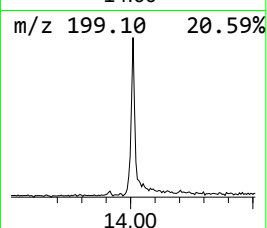
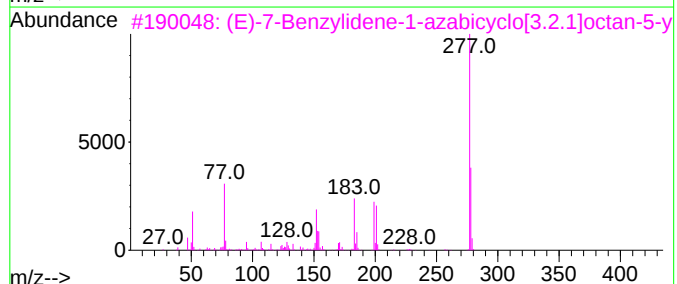
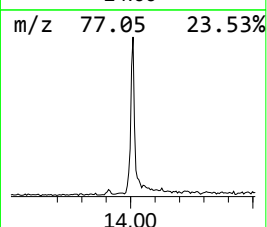
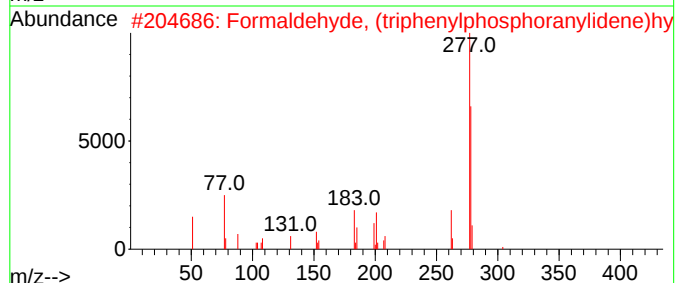
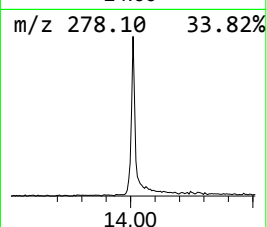
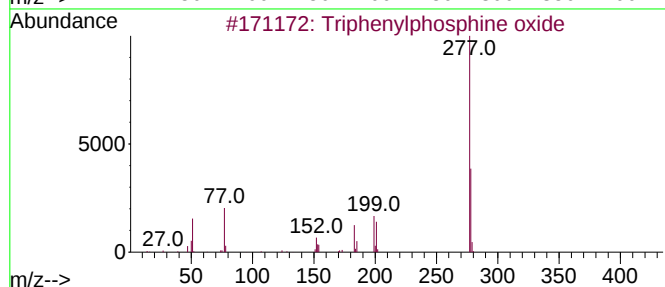
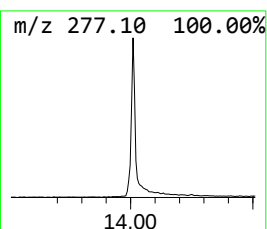
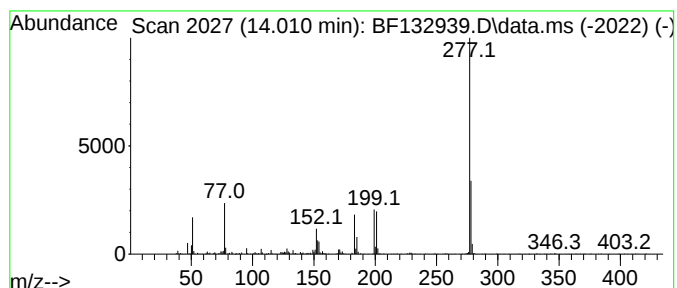
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.010	7.36 ng	618632	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	58
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	6.0	ng	571317	1	6.757	1896670	20.0
Benzophenone	10.510	2.9	ng	375980	3	9.798	2610030	20.0
n-Hexadecanoic ...	11.816	4.7	ng	546334	4	11.281	2336310	20.0
17-Pentatriacon...	13.775	6.8	ng	575338	5	13.916	1682080	20.0
Triphenylphosph...	14.010	7.4	ng	618632	5	13.916	1682080	20.0