

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
 Data File : BM049882.D
 Acq On : 10 Apr 2025 13:31
 Operator : RC/JU
 Sample : Q1752-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-4

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_M\Methods\8270-BM040825.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049882.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	319	324	334	rVB	986406	1310990	10.09%	1.987%
2	5.357	397	403	414	rBV	4172608	6015686	46.28%	9.116%
3	5.969	502	507	515	rVB	156459	225952	1.74%	0.342%
4	6.951	666	674	689	rBV	3953167	6139143	47.23%	9.303%
5	7.775	807	814	823	rBV	948918	1456341	11.20%	2.207%
6	8.928	1003	1010	1022	rBV	2273723	3787871	29.14%	5.740%
7	10.569	1280	1289	1301	rBV	1092241	1839655	14.15%	2.788%
8	13.039	1702	1709	1724	rBV	6243663	8667319	66.68%	13.135%
9	14.416	1935	1943	1950	rBV	1750323	2495386	19.20%	3.782%
10	15.774	2167	2174	2181	rBV	1341633	1769891	13.62%	2.682%
11	15.904	2189	2196	2213	rBV	5450173	7763756	59.73%	11.765%
12	16.339	2263	2270	2275	rBV	100678	132135	1.02%	0.200%
13	17.162	2402	2410	2416	rBV2	2074157	2969805	22.85%	4.500%
14	18.062	2557	2563	2572	rBV	535971	851045	6.55%	1.290%
15	19.339	2776	2780	2788	rBV	160292	251300	1.93%	0.381%
16	19.786	2850	2856	2867	rBV	11489094	12997500	100.00%	19.697%
17	21.080	3072	3076	3085	rBV2	233232	422846	3.25%	0.641%
18	21.392	3124	3129	3135	rBV	2261465	3299448	25.39%	5.000%
19	24.391	3631	3639	3657	rVB	1396512	3592783	27.64%	5.445%

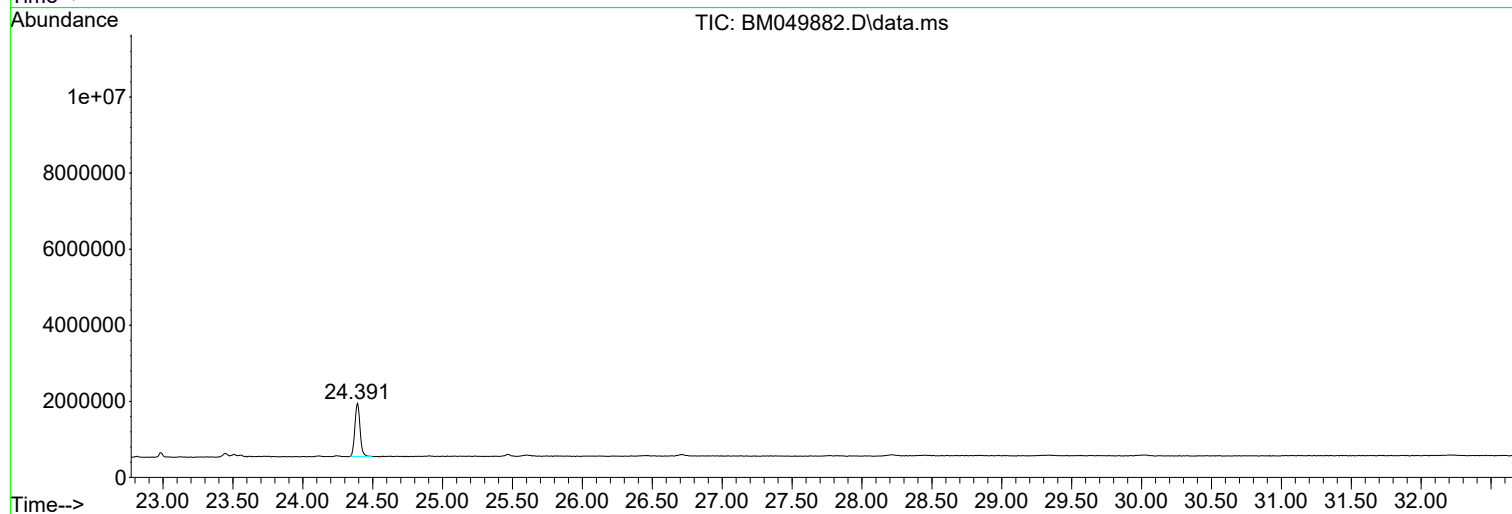
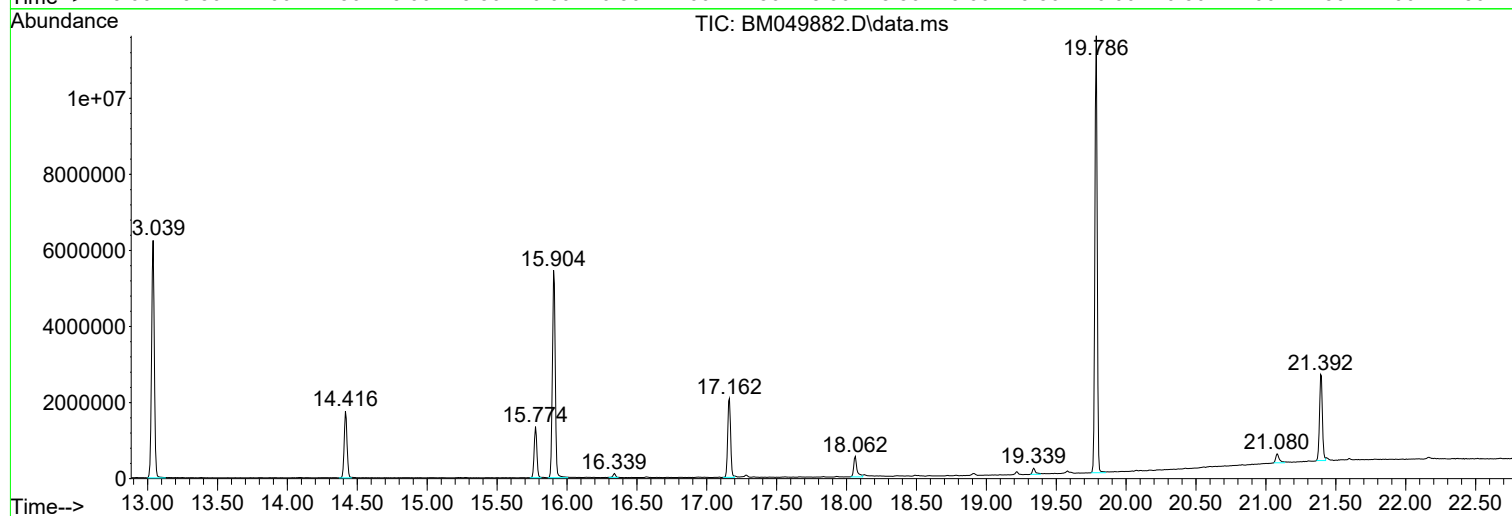
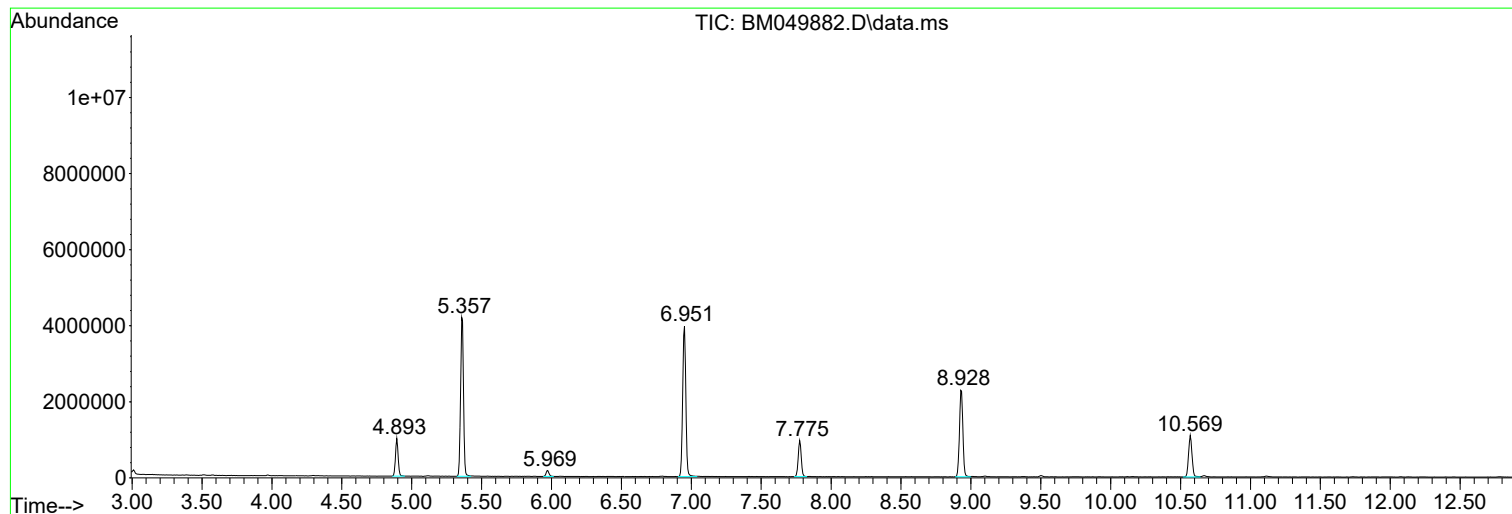
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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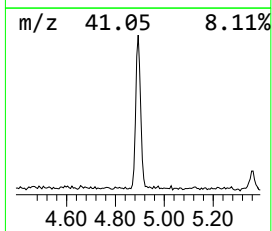
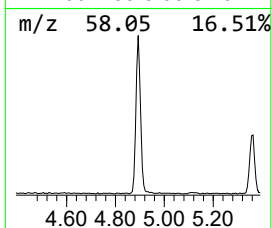
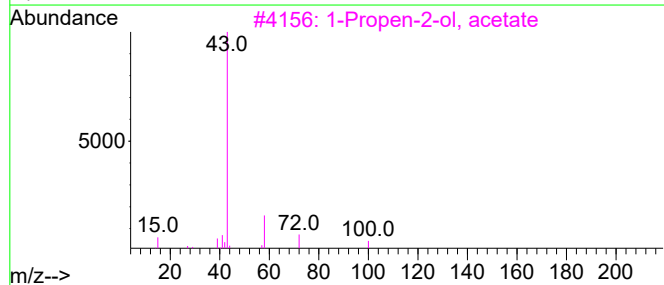
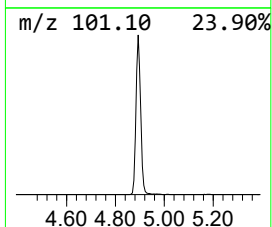
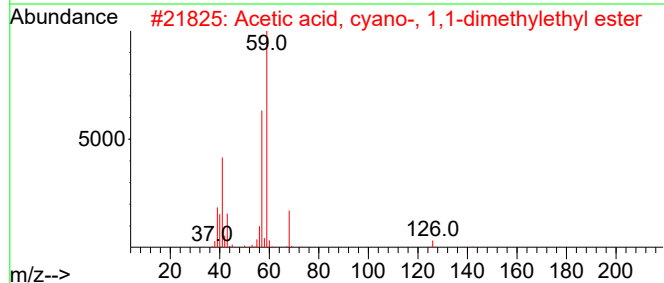
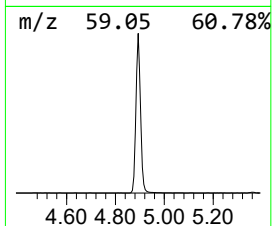
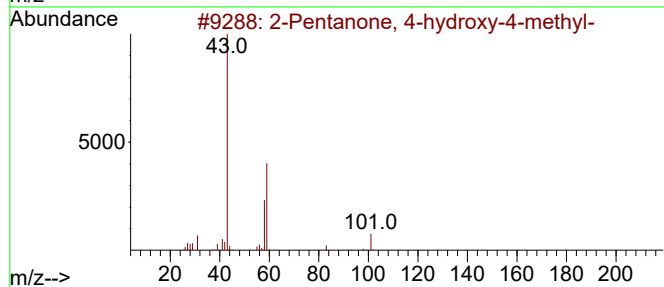
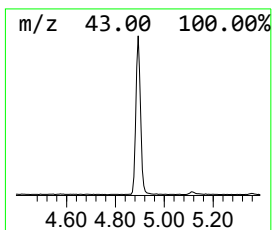
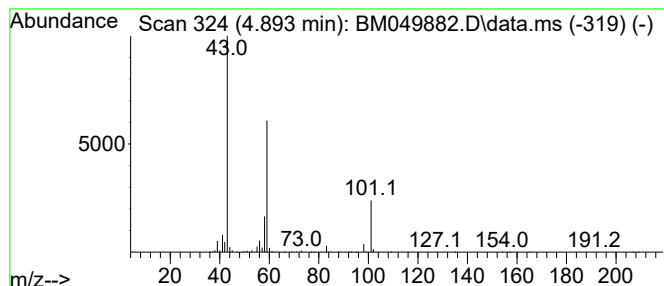
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.893	18.00 ng	1310990	1,4-Dichlorobenzene-d4	7.775

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	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Guanidine	59	CH5N3	000113-00-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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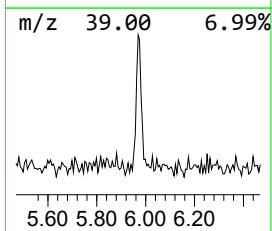
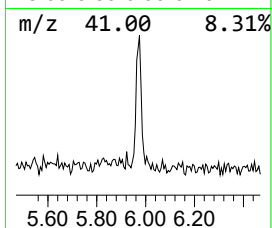
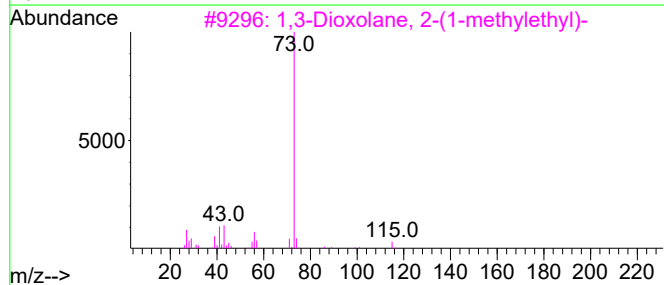
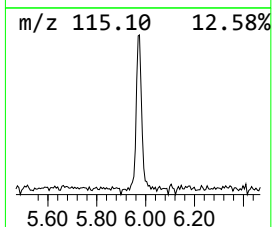
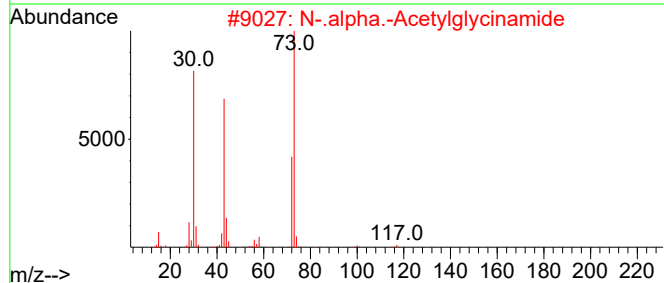
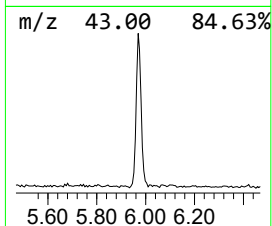
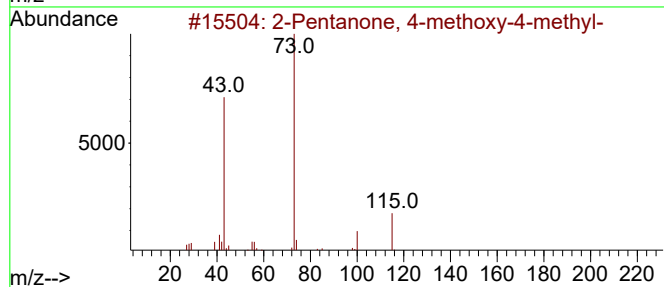
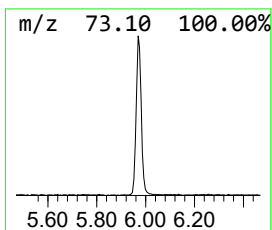
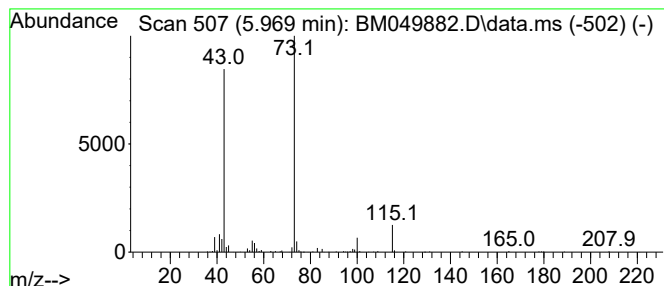
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	3.10 ng	225952	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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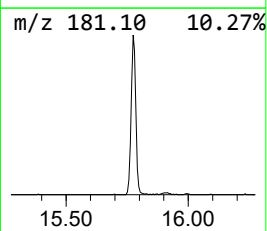
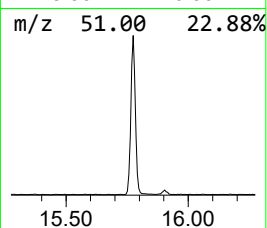
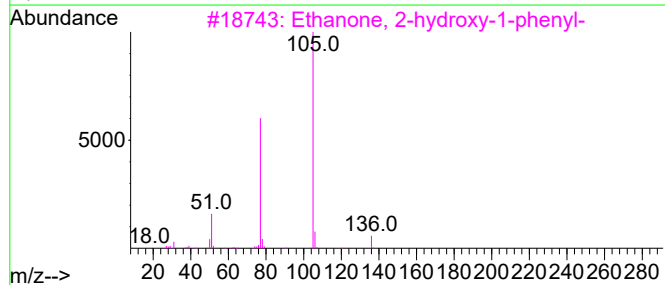
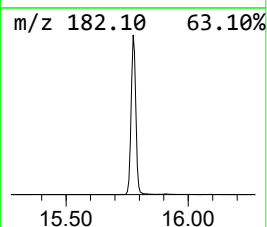
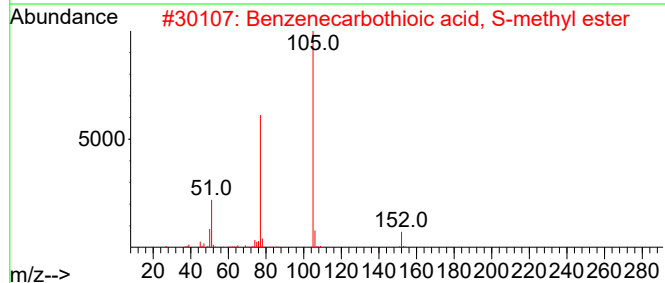
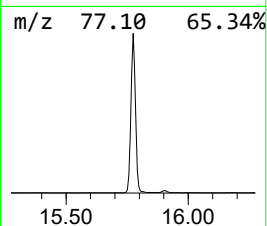
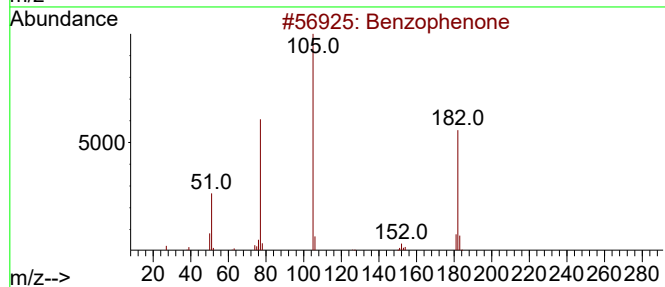
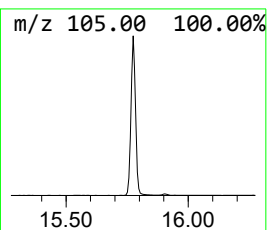
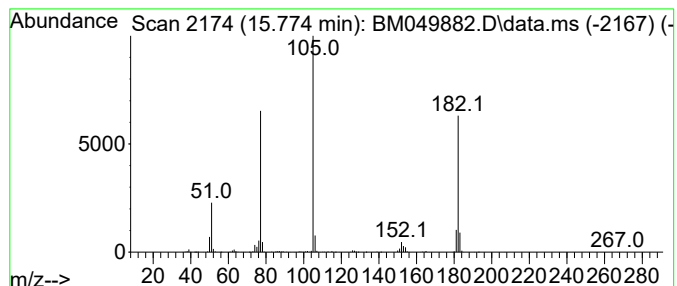
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	14.19 ng	1769890	Acenaphthene-d10	14.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	43
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	43



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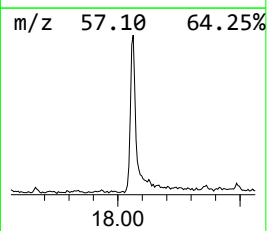
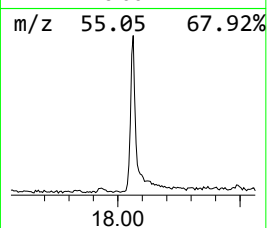
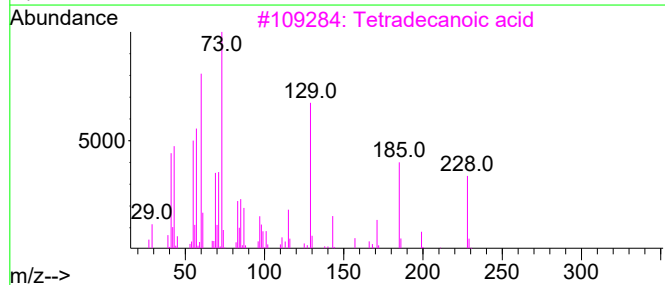
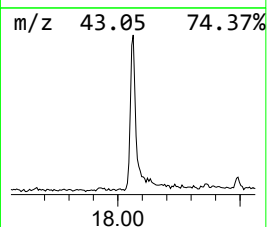
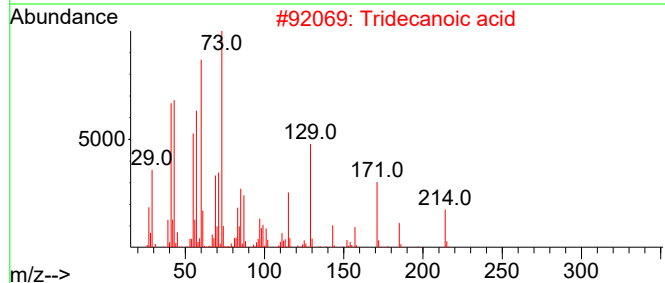
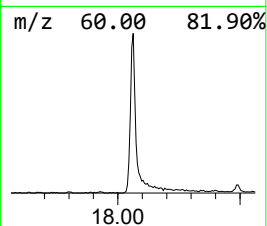
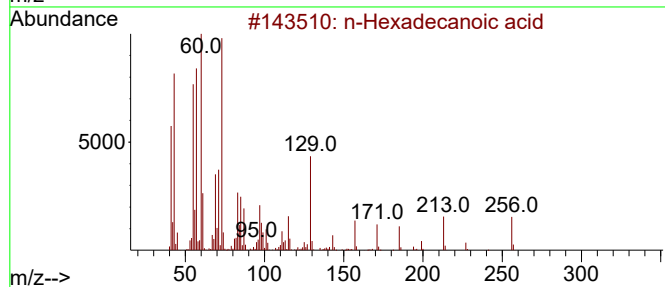
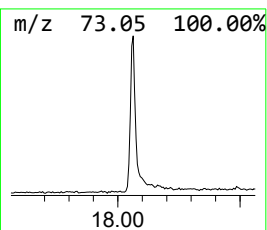
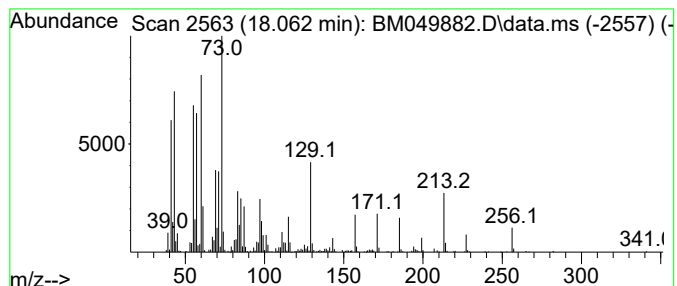
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	5.73 ng	851045	Phenanthrene-d10	17.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	80



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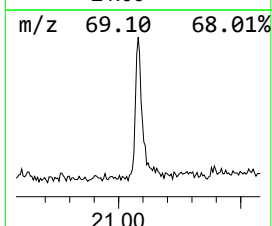
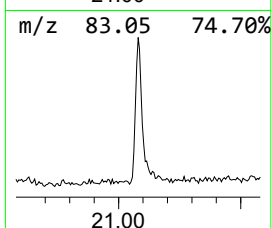
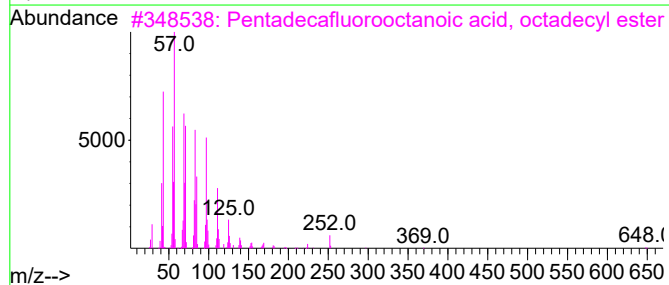
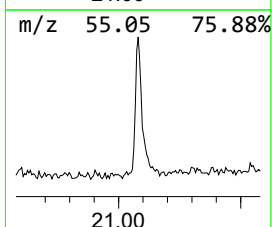
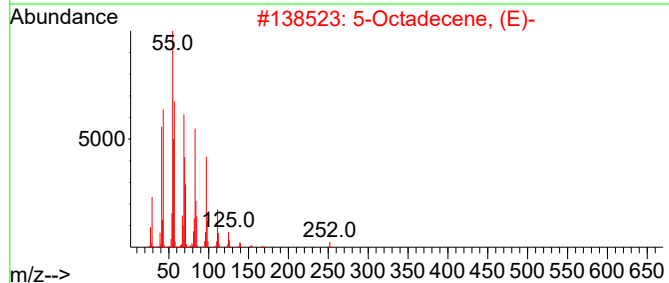
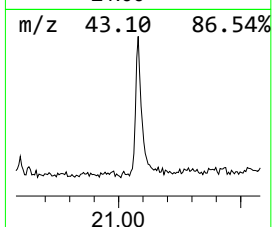
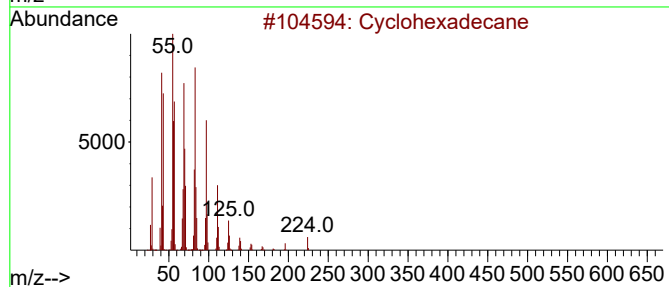
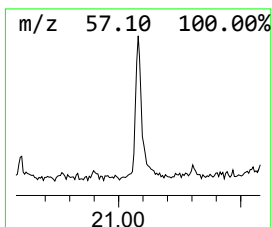
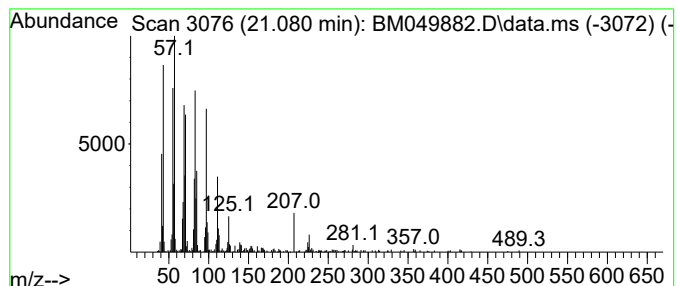
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	2.56 ng	422846	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	93
5			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	90



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.893	18.0	ng	1310990	1	7.775	1456340	20.0
2-Pentanone, 4-...	5.969	3.1	ng	225952	1	7.775	1456340	20.0
Benzophenone	15.774	14.2	ng	1769890	3	14.416	2495390	20.0
n-Hexadecanoic ...	18.062	5.7	ng	851045	4	17.163	2969810	20.0
Cyclohexadecane	21.080	2.6	ng	422846	5	21.392	3299450	20.0