

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043025\
 Data File : BM050048.D
 Acq On : 30 Apr 2025 16:44
 Operator : RC/JU
 Sample : Q1883-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OU4-PCS-TC-31-042325

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-BM042825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	318	323	338	rVB	403077	582414	3.10%	0.780%
2	5.357	396	403	422	rBV	4191871	6463524	34.45%	8.662%
3	6.945	665	673	702	rBV	3809011	6854638	36.53%	9.186%
4	7.763	804	812	824	rBV	804260	1327252	7.07%	1.779%
5	8.922	1001	1009	1030	rBV	2316327	4201689	22.39%	5.631%
6	10.563	1280	1288	1304	rBV	842399	1683667	8.97%	2.256%
7	13.027	1699	1707	1725	rBV	7688138	11339799	60.43%	15.196%
8	14.410	1935	1942	1958	rBV	1510324	2401717	12.80%	3.219%
9	15.768	2167	2173	2189	rBV	1479746	2107989	11.23%	2.825%
10	15.904	2189	2196	2220	rVV	5870165	8997078	47.95%	12.057%
11	16.333	2263	2269	2278	rBV	218752	342513	1.83%	0.459%
12	17.156	2403	2409	2424	rBV	1717231	2763677	14.73%	3.704%
13	18.050	2556	2561	2571	rBV	243356	443440	2.36%	0.594%
14	19.780	2849	2855	2866	rBV	16634038	18763786	100.00%	25.145%
15	21.074	3071	3075	3086	rVB2	229114	428079	2.28%	0.574%
16	21.397	3124	3130	3144	rBV	1837559	2928121	15.61%	3.924%
17	24.397	3632	3640	3654	rVB	1136483	2992312	15.95%	4.010%

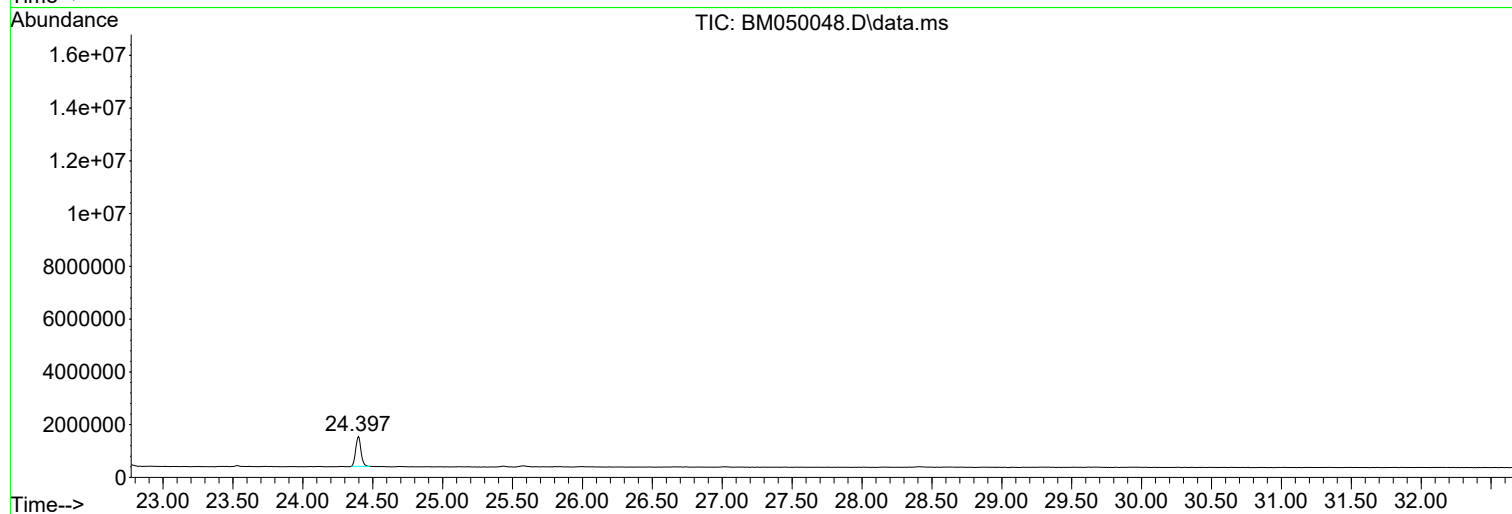
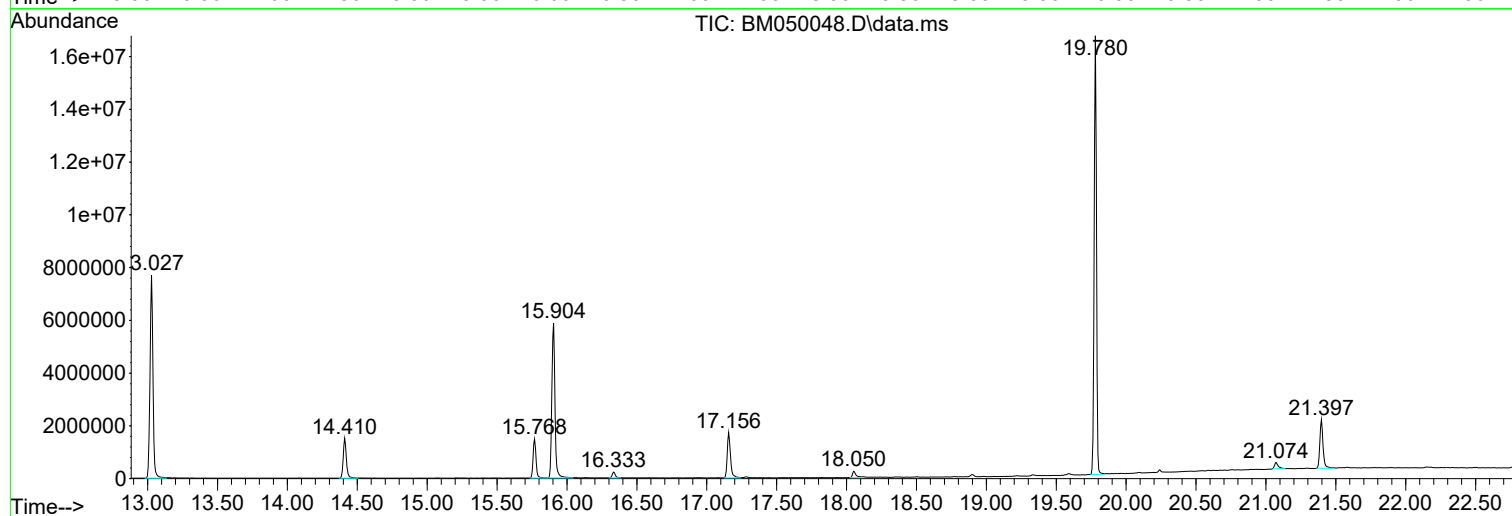
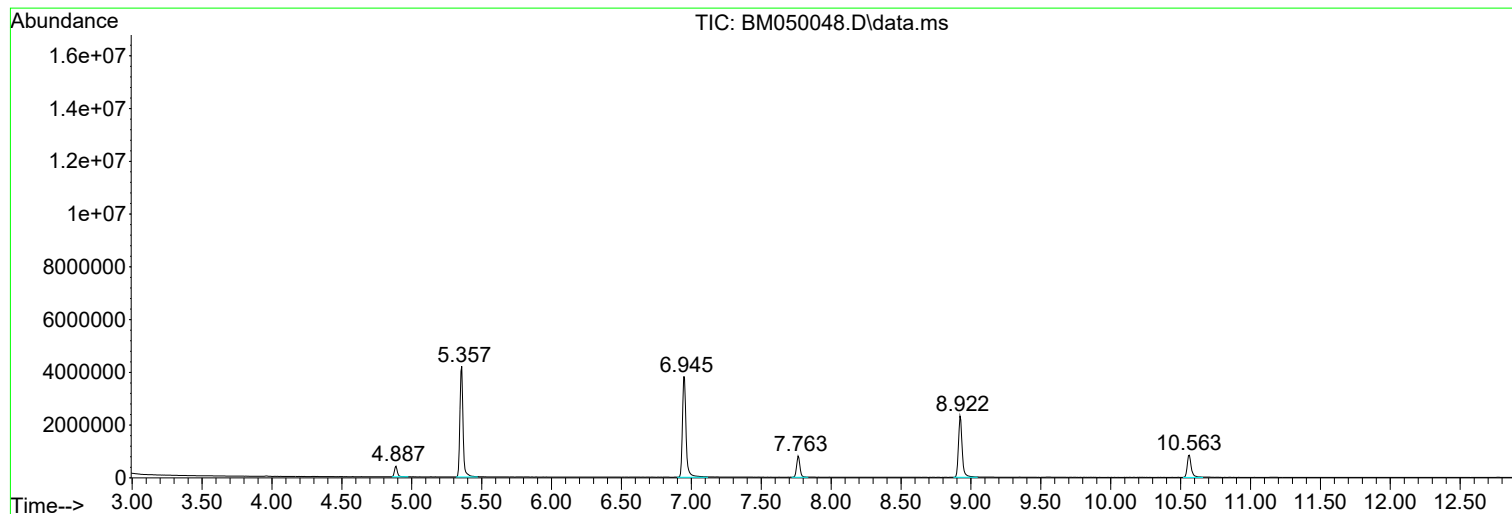
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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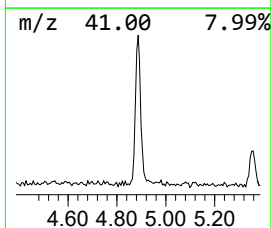
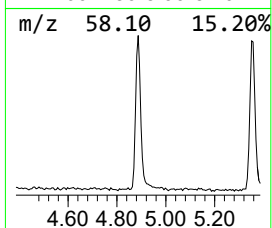
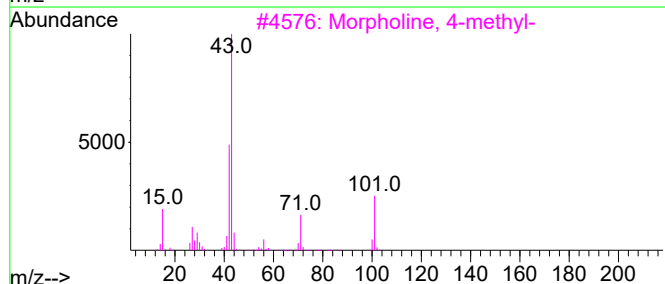
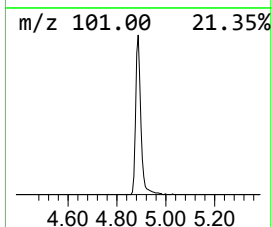
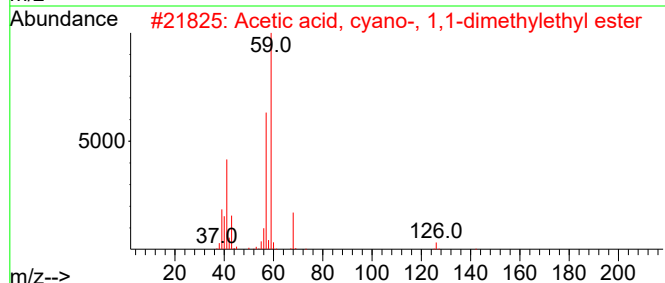
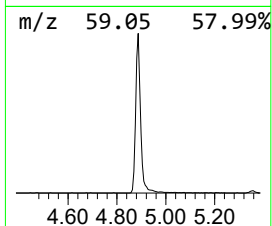
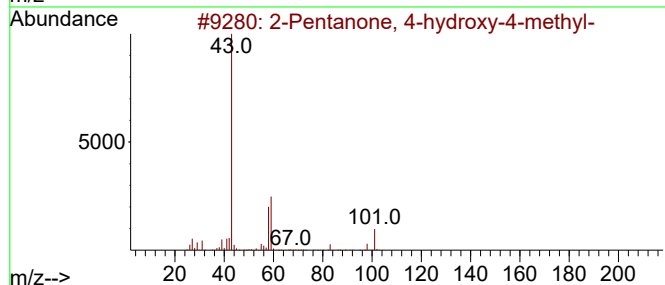
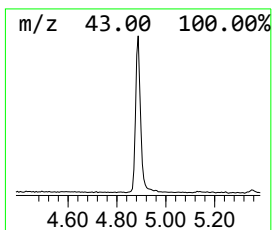
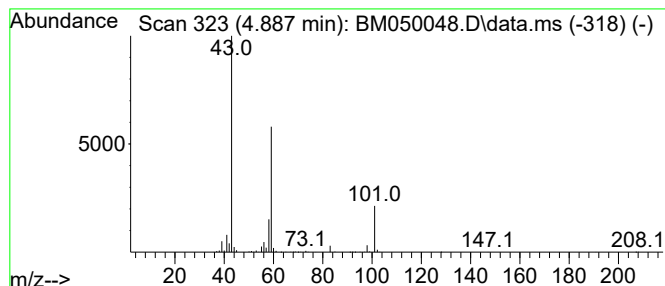
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	8.78 ng	582414	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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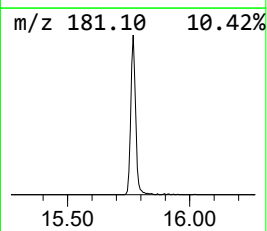
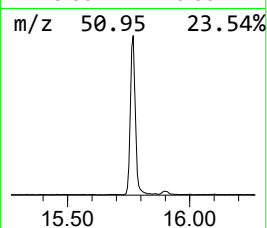
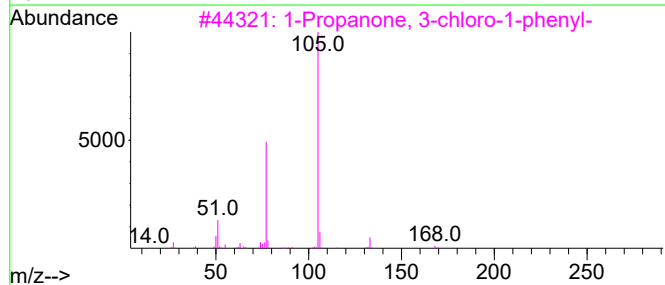
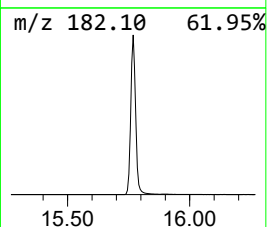
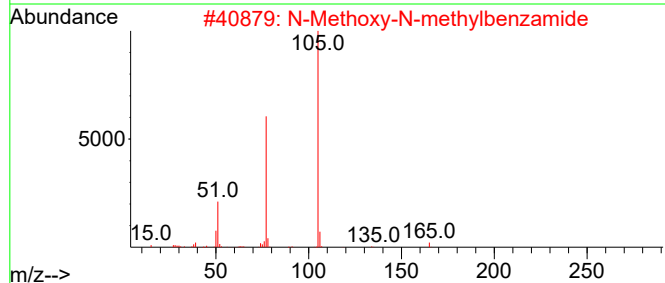
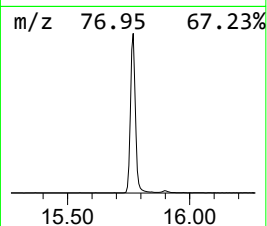
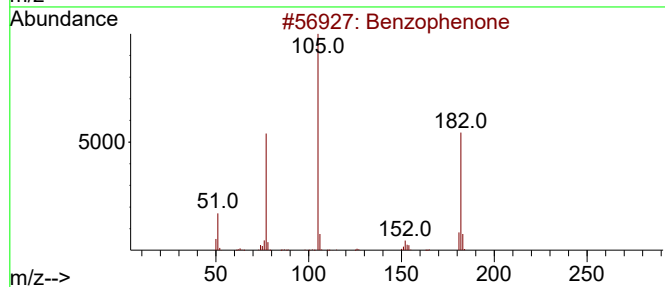
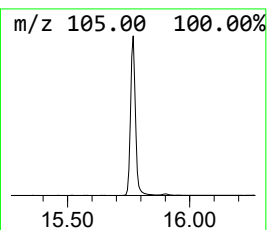
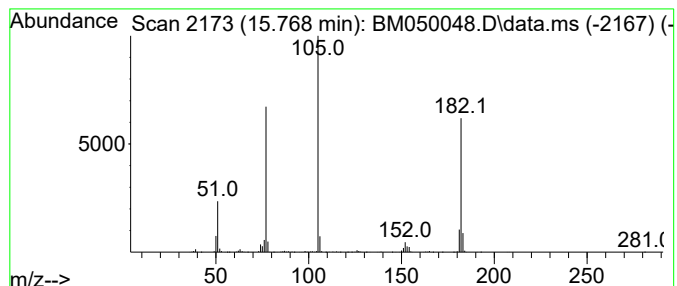
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	17.55 ng	2107990	Acenaphthene-d10	14.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



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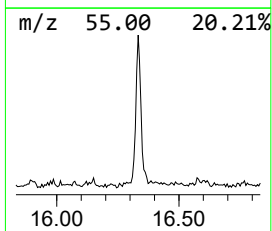
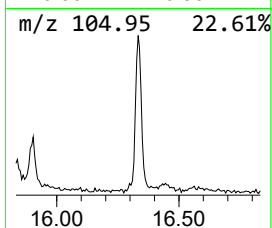
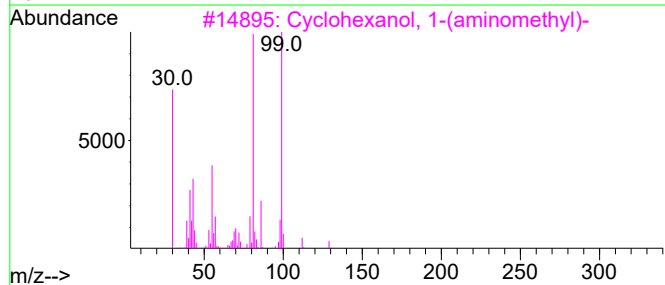
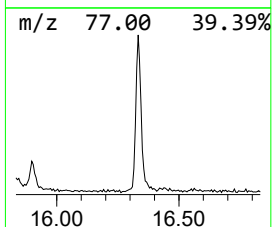
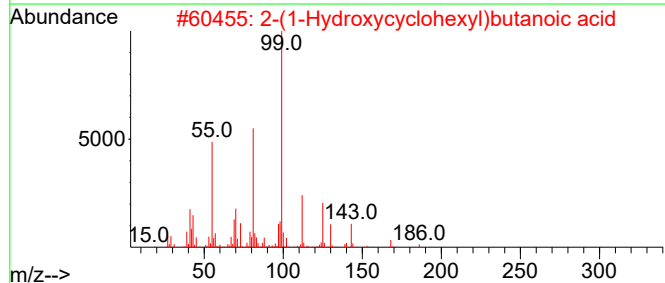
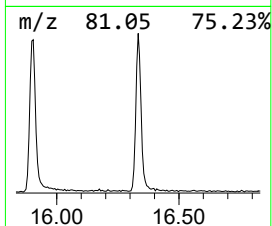
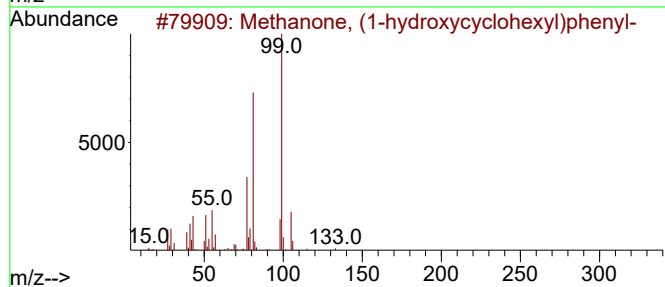
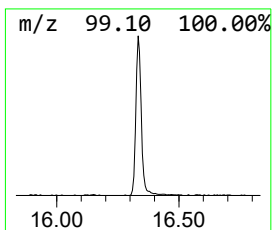
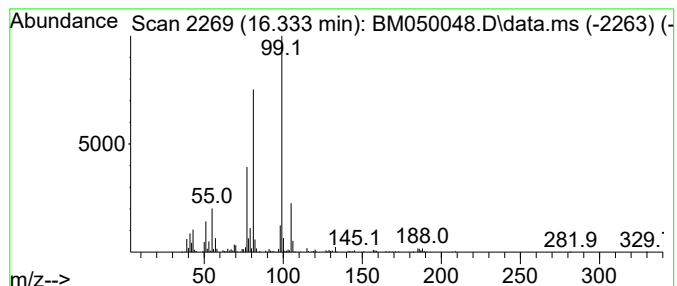
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.333	2.48 ng	342513	Phenanthrene-d10		17.156	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...		204	C13H16O2	000947-19-3	90
2	2-(1-Hydroxycyclohexyl)butanoic ...		186	C10H18O3	000512-16-3	53
3	Cyclohexanol, 1-(aminomethyl)-		129	C7H15NO	004000-72-0	53
4	3-Methylcyclohexyl methylphospho...		194	C8H16FO2P	113548-86-0	50
5	Cyclohexanol, 1-ethyl-		128	C8H16O	001940-18-7	50



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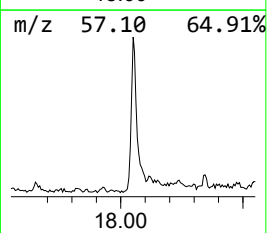
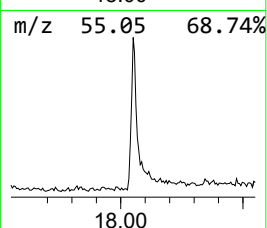
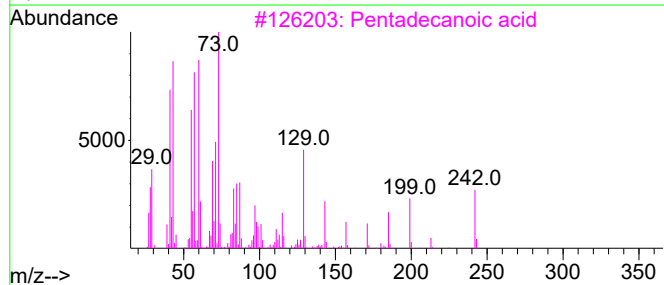
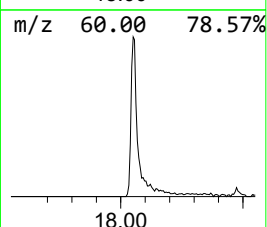
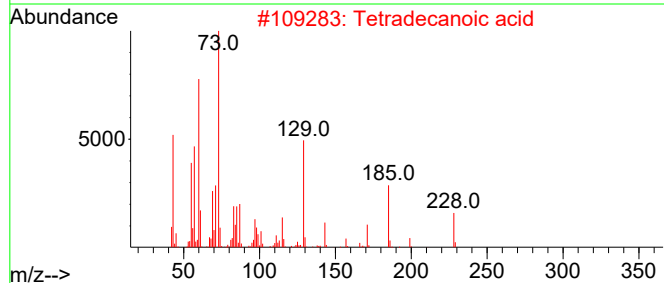
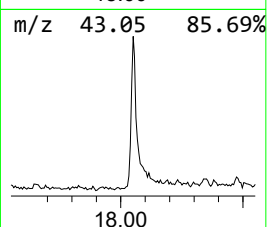
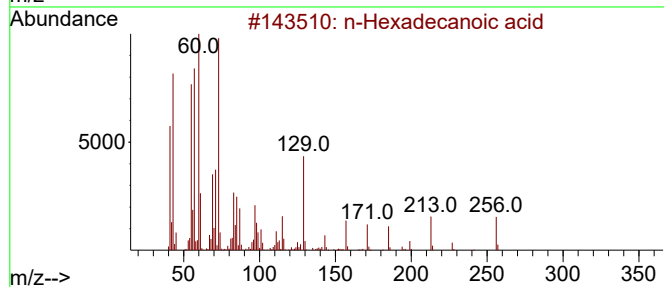
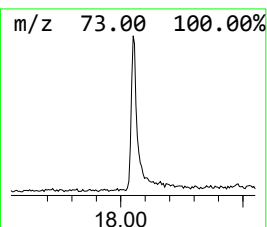
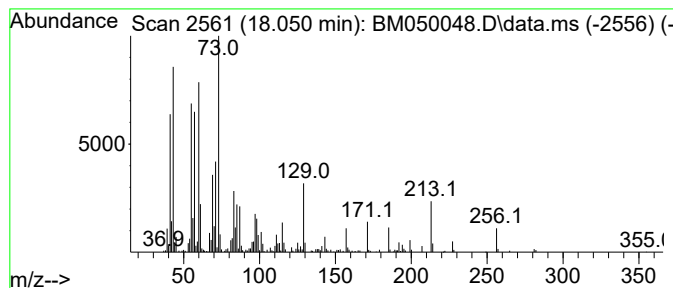
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.051	3.21 ng	443440	Phenanthrene-d10	17.156

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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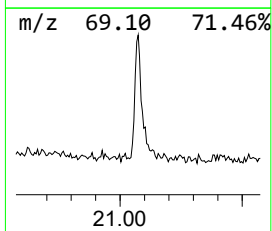
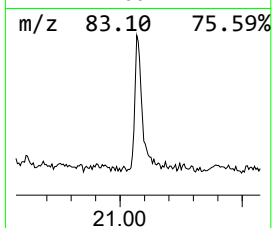
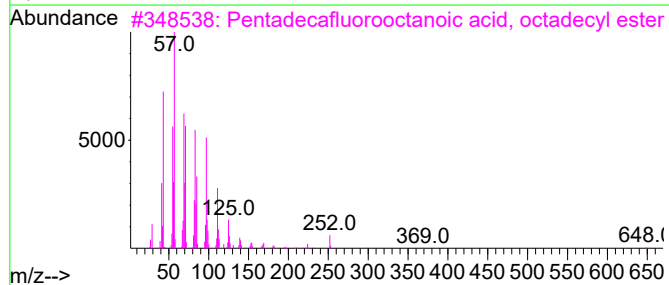
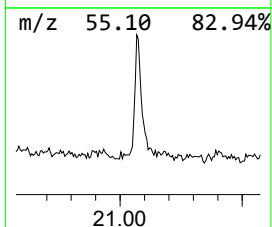
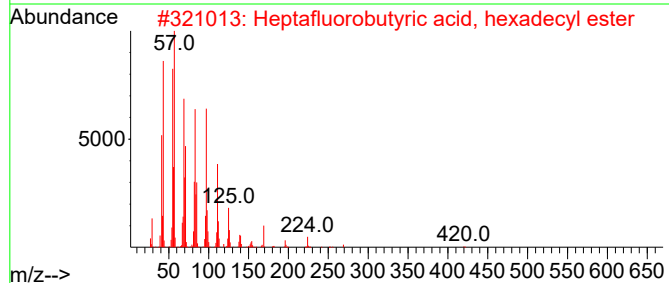
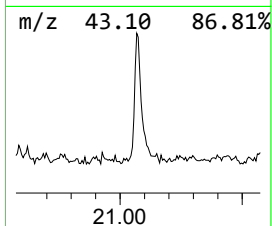
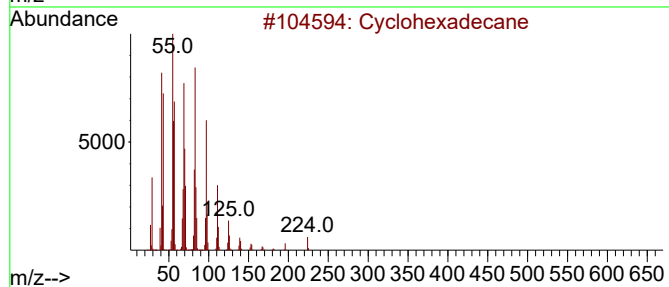
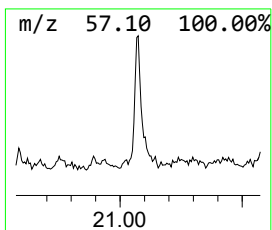
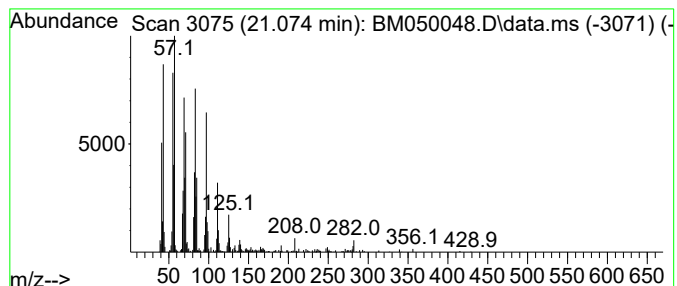
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Peak Number 5 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	2.92 ng	428079	Chrysene-d12	21.397

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	96
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.887	8.8	ng	582414	1	7.763	1327250	20.0
Benzophenone	15.768	17.6	ng	2107990	3	14.410	2401720	20.0
Methanone, (1-h...	16.333	2.5	ng	342513	4	17.156	2763680	20.0
n-Hexadecanoic ...	18.051	3.2	ng	443440	4	17.156	2763680	20.0
Cyclohexadecane	21.074	2.9	ng	428079	5	21.397	2928120	20.0