

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057844.D
 Acq On : 23 Jun 2023 16:04
 Operator : CG/JU
 Sample : 03336-10
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-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_G\Methods\8270-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057844.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.026	322	330	338	rVB	58674	85777	3.65%	0.678%
2	5.490	403	409	423	rVB	687341	1092740	46.49%	8.641%
3	7.083	672	680	689	rBV	726039	1211706	51.56%	9.582%
4	7.917	815	822	829	rBV	148010	247056	10.51%	1.954%
5	9.080	1012	1020	1028	rBV	413958	716415	30.48%	5.665%
6	10.725	1292	1300	1308	rVB	219154	390108	16.60%	3.085%
7	13.176	1710	1717	1728	rVB	1037088	1620015	68.93%	12.811%
8	14.556	1945	1952	1960	rVB	372465	581578	24.75%	4.599%
9	15.908	2174	2182	2188	rBV	116186	161137	6.86%	1.274%
10	16.043	2198	2205	2217	rBV	928125	1426930	60.71%	11.284%
11	17.300	2412	2419	2425	rBV	466446	701538	29.85%	5.548%
12	18.187	2563	2570	2576	rBV	90577	139109	5.92%	1.100%
13	19.456	2781	2786	2792	rBV2	25310	42487	1.81%	0.336%
14	19.915	2858	2864	2870	rBV	1783559	2350235	100.00%	18.585%
15	21.201	3079	3083	3093	rBV	101882	151189	6.43%	1.196%
16	21.548	3136	3142	3154	rVB2	458614	734559	31.25%	5.809%
17	22.359	3274	3280	3286	rBV7	31176	73382	3.12%	0.580%
18	22.988	3385	3387	3396	rVB7	19057	42375	1.80%	0.335%
19	23.804	3523	3526	3533	rVB3	19478	37269	1.59%	0.295%
20	24.697	3668	3678	3694	rVB	296185	840093	35.75%	6.643%

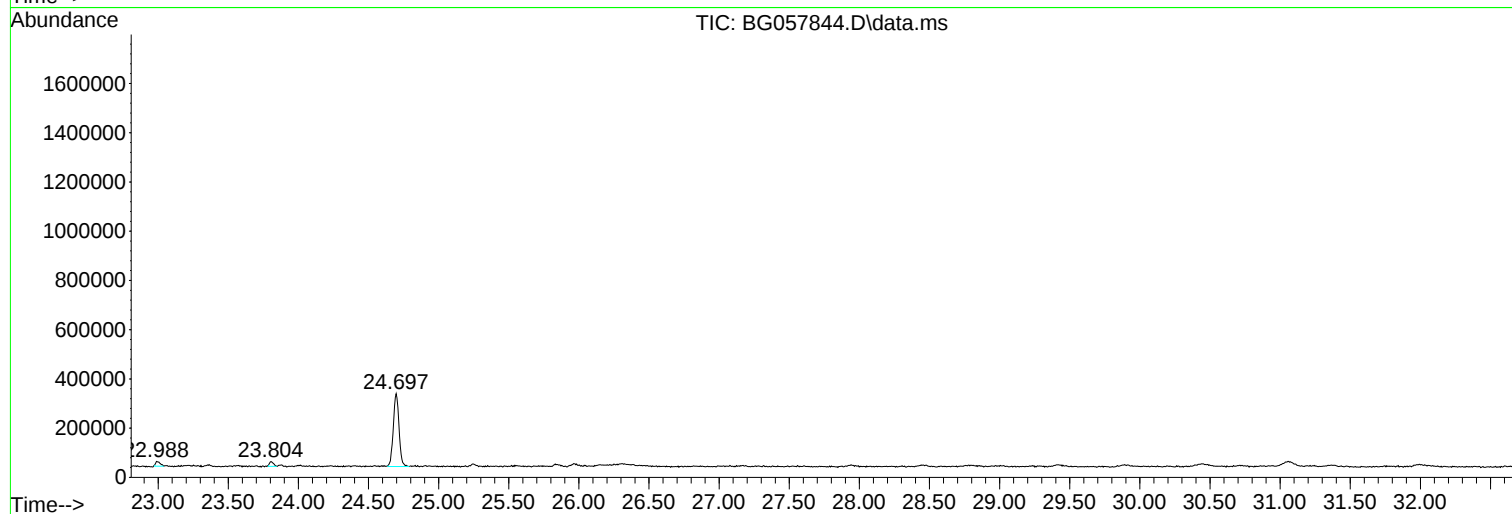
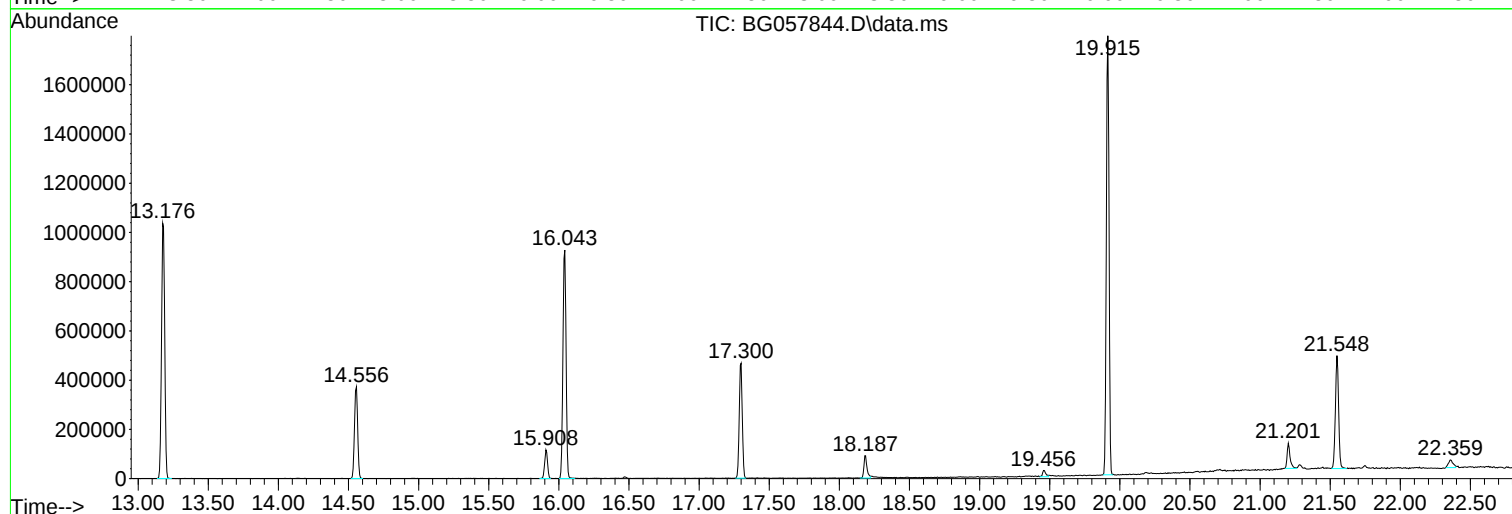
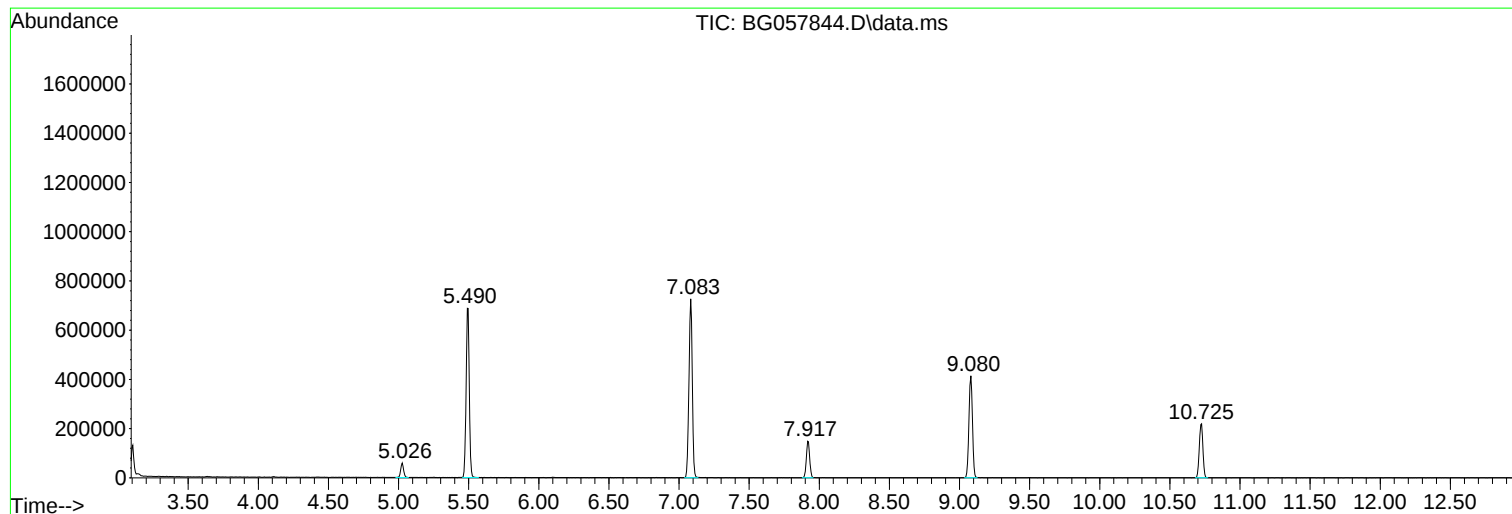
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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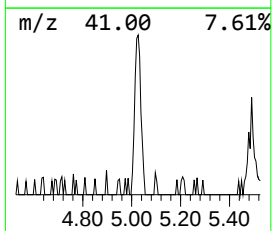
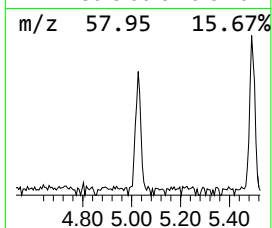
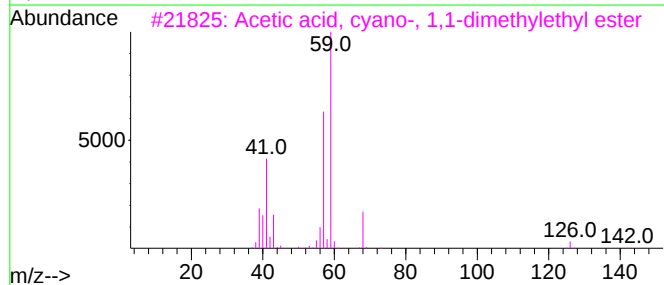
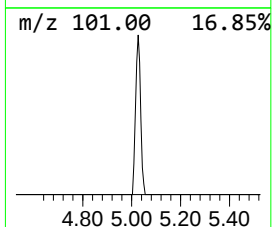
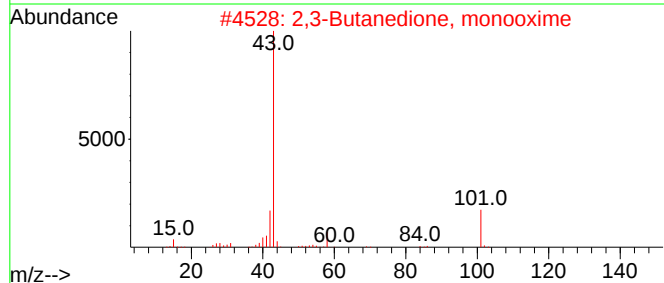
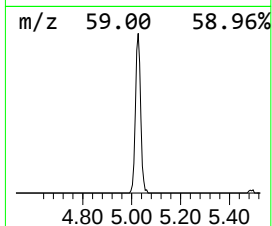
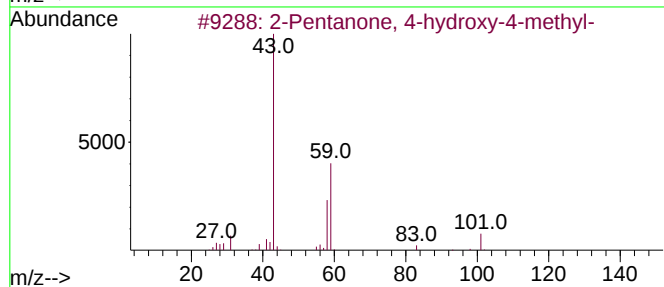
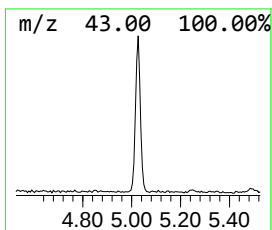
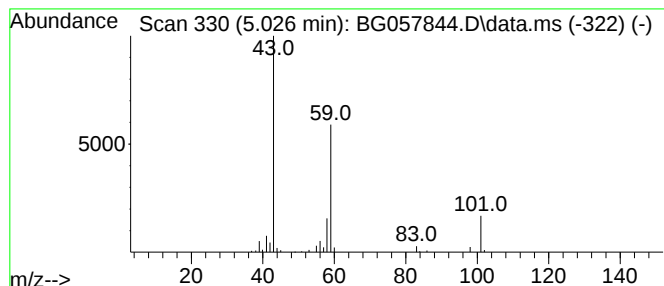
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.026	6.94 ng	85777	1,4-Dichlorobenzene-d4	7.923

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37		
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		



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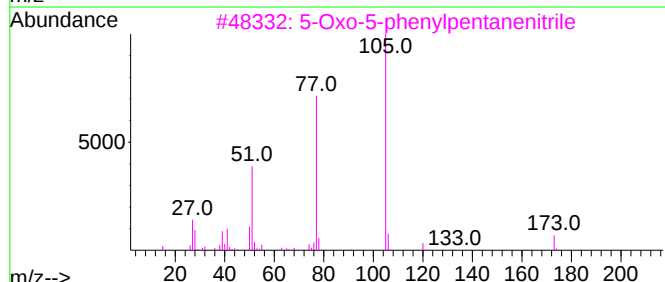
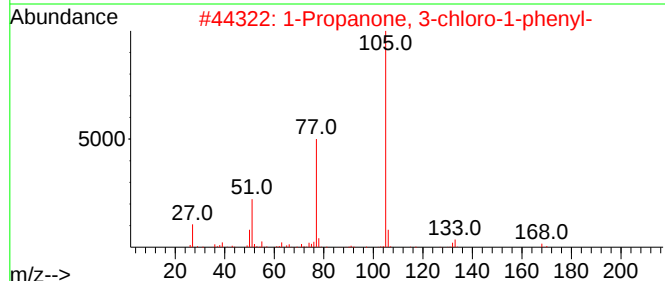
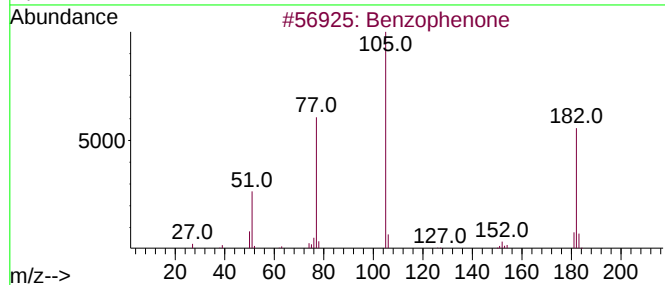
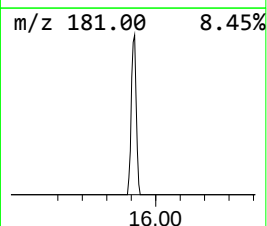
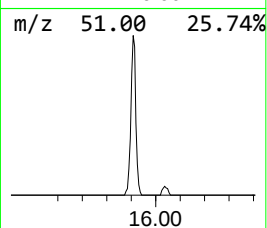
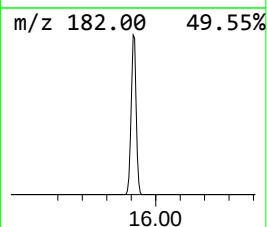
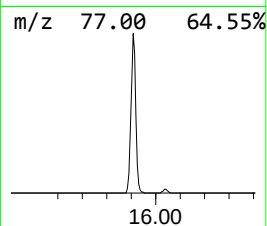
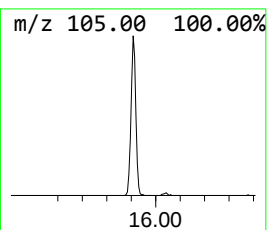
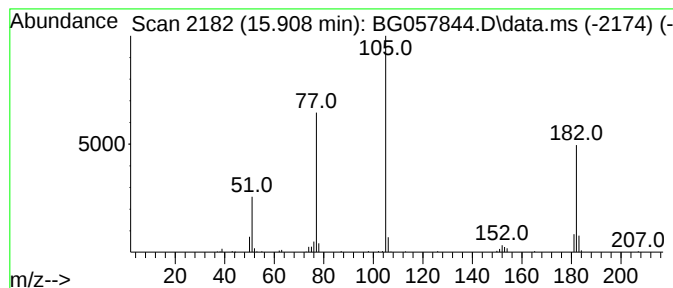
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	5.54 ng	161137	Acenaphthene-d10	14.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	47
4			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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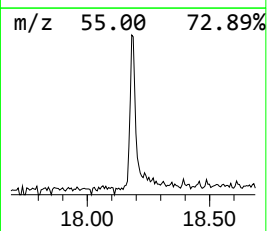
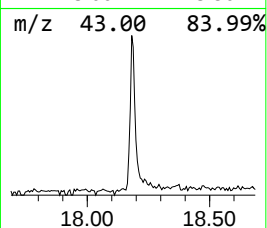
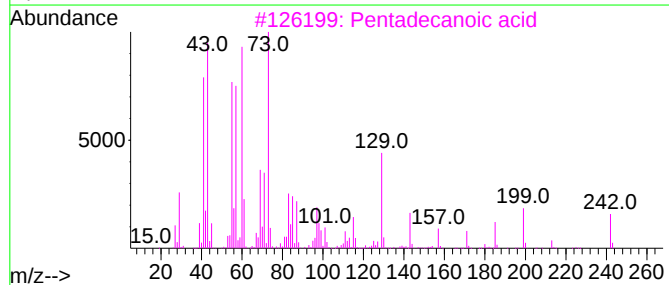
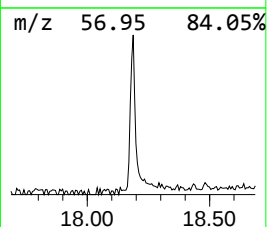
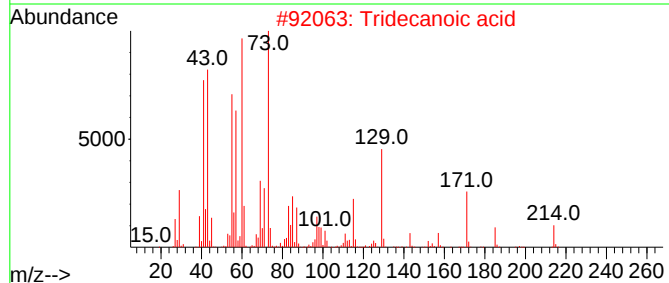
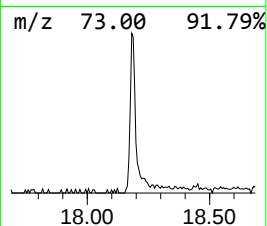
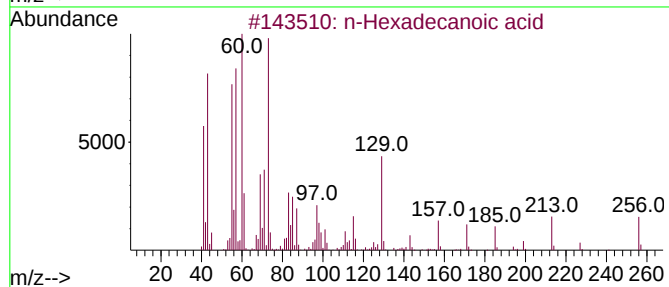
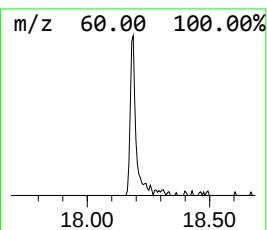
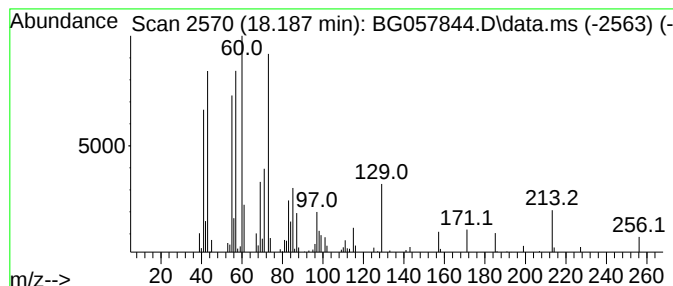
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.187	3.97 ng	139109	Phenanthrene-d10	17.300

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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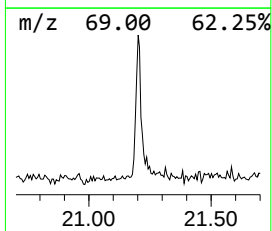
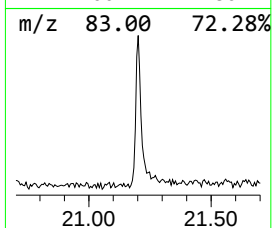
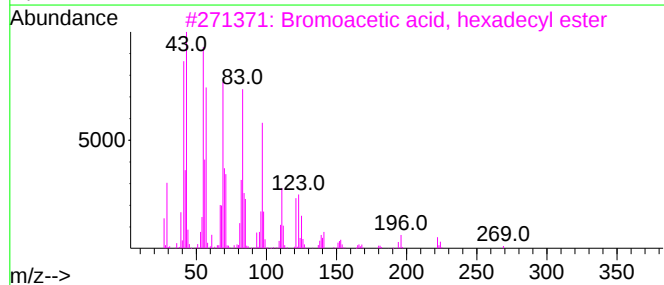
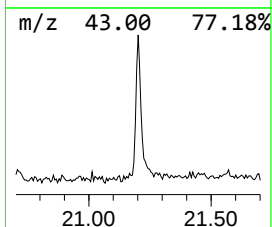
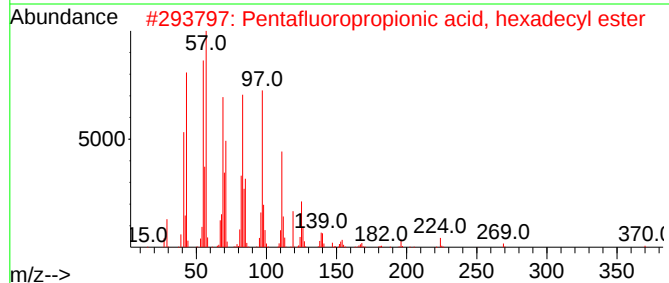
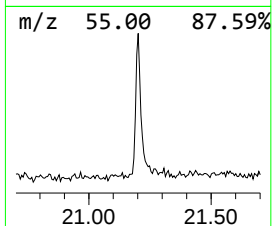
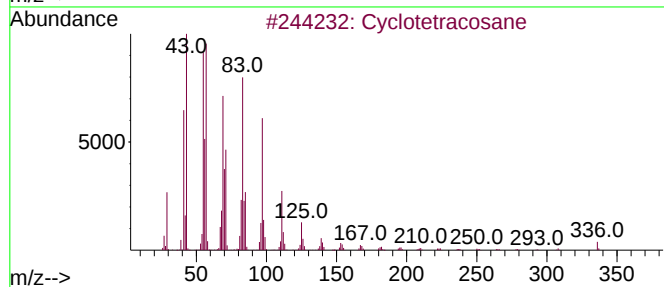
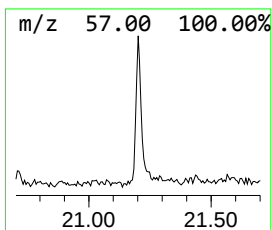
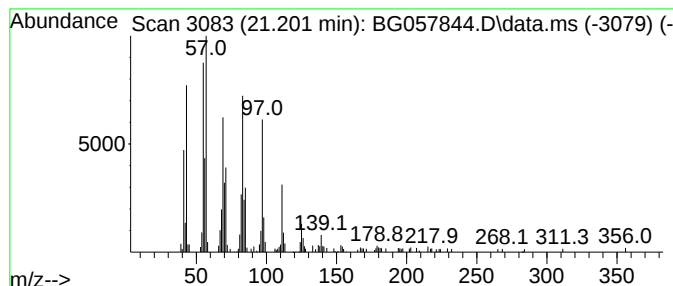
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Peak Number 4 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.201	4.12 ng	151189	Chrysene-d12	21.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	95
2			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
3			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4			1-Hexacosene	364	C26H52	018835-33-1	91
5			Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.026	6.9	ng	85777	1	7.923	247056	20.0
Benzophenone	15.908	5.5	ng	161137	3	14.556	581578	20.0
n-Hexadecanoic ...	18.187	4.0	ng	139109	4	17.300	701538	20.0
Cyclotetracosane	21.201	4.1	ng	151189	5	21.548	734559	20.0