

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121423\
 Data File : BG060023.D
 Acq On : 14 Dec 2023 22:25
 Operator : MA/JU
 Sample : 05631-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-2A

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060023.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	4	9	26	rVB	581319	996245	8.11%	2.090%
2	5.061	330	336	342	rBV2	195041	294345	2.40%	0.618%
3	5.525	408	415	424	rVB	1619965	2541177	20.69%	5.331%
4	7.112	677	685	697	rBV	1469002	2420897	19.71%	5.079%
5	7.952	822	828	837	rBV	370241	642419	5.23%	1.348%
6	9.121	1018	1027	1036	rVB	1637014	2959814	24.10%	6.210%
7	10.760	1296	1306	1312	rBV	471653	851780	6.93%	1.787%
8	13.222	1716	1725	1732	rVB	5082054	7975144	64.93%	16.732%
9	14.380	1915	1922	1928	rBV3	97798	158354	1.29%	0.332%
10	14.591	1951	1958	1965	rBV	886415	1387492	11.30%	2.911%
11	16.084	2204	2212	2218	rBV	5636853	8082771	65.80%	16.958%
12	16.736	2318	2323	2330	rBV5	97375	175847	1.43%	0.369%
13	17.341	2419	2426	2433	rVB	1237677	1869200	15.22%	3.922%
14	18.234	2572	2578	2589	rBV2	465189	689173	5.61%	1.446%
15	19.509	2791	2795	2800	rBV2	163150	202354	1.65%	0.425%
16	19.967	2866	2873	2878	rBV	9013676	12283274	100.00%	25.770%
17	21.607	3146	3152	3159	rBV2	1249004	1999993	16.28%	4.196%
18	24.797	3685	3695	3707	rVB	761832	2134211	17.37%	4.478%

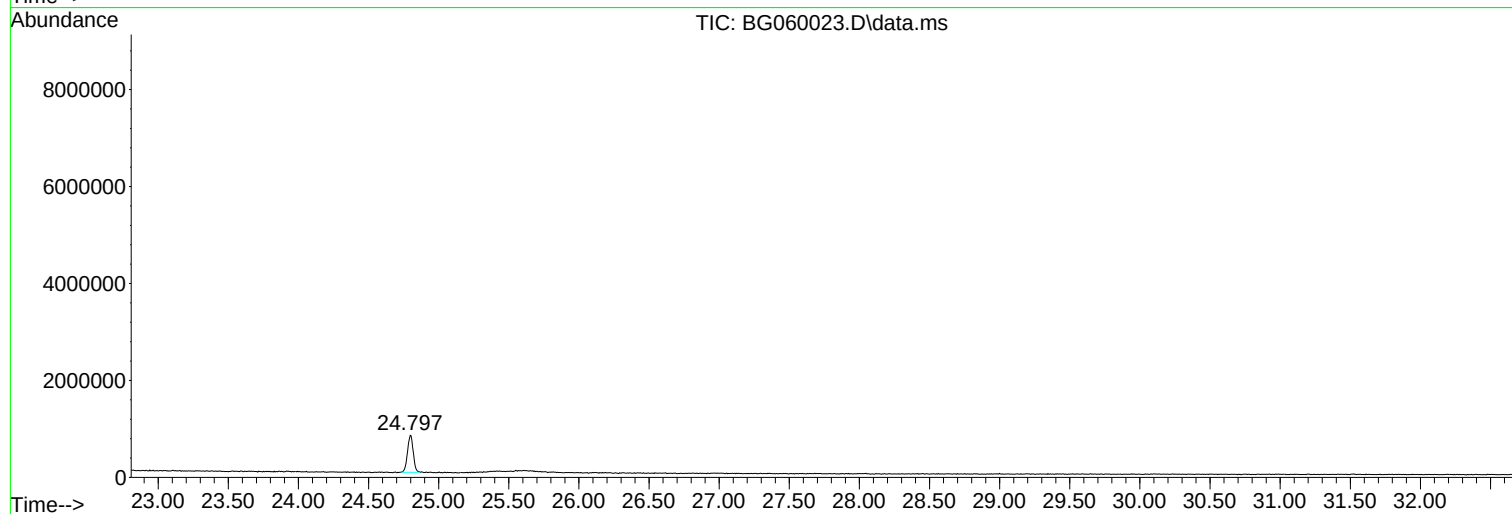
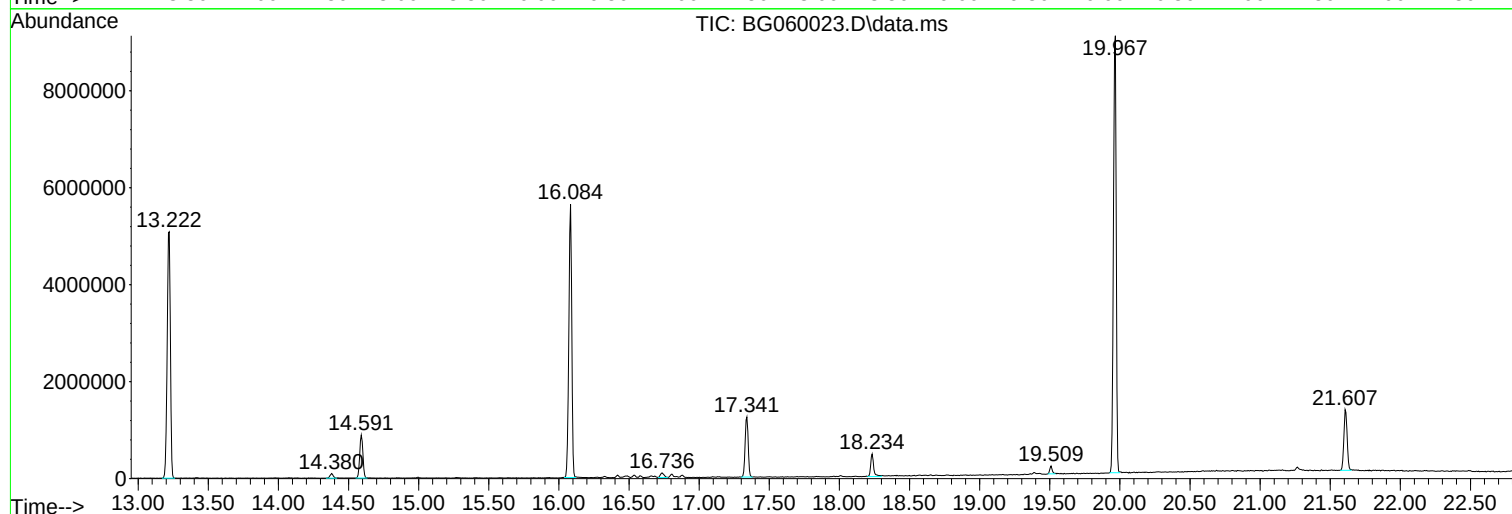
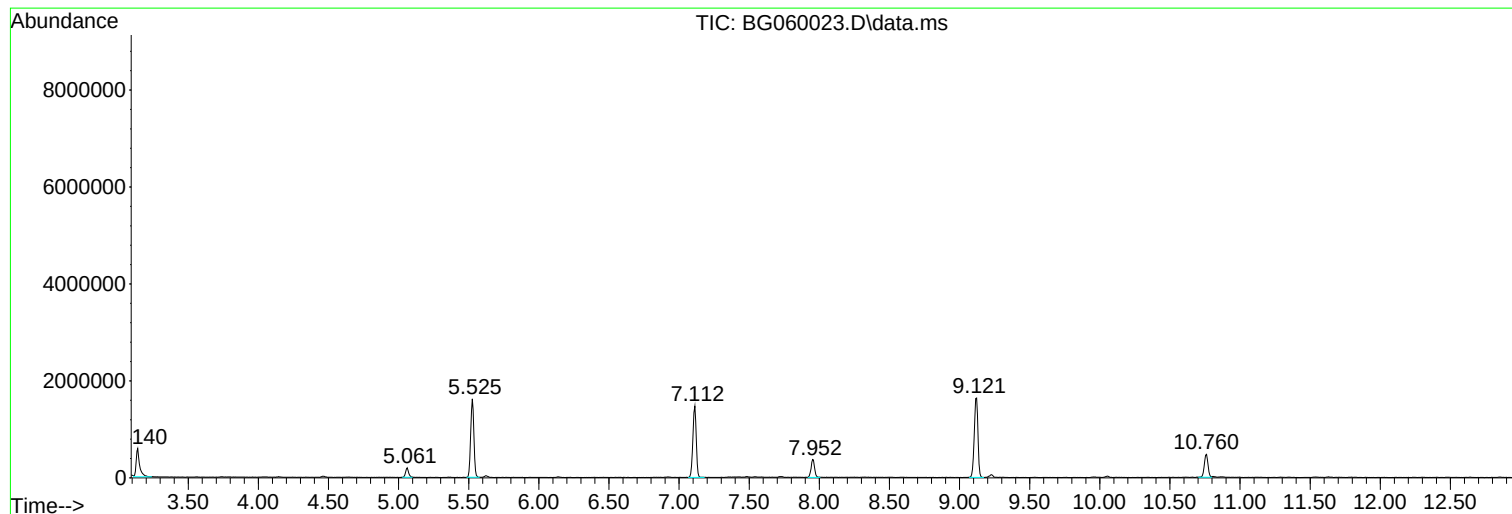
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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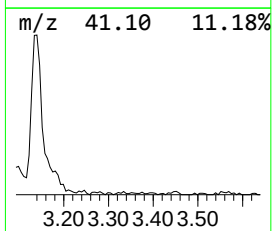
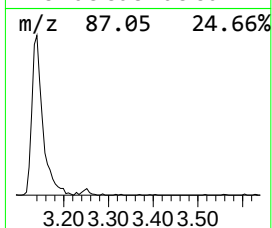
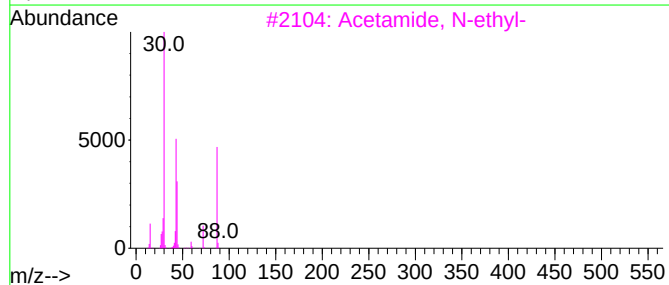
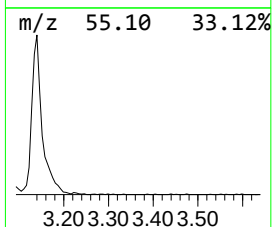
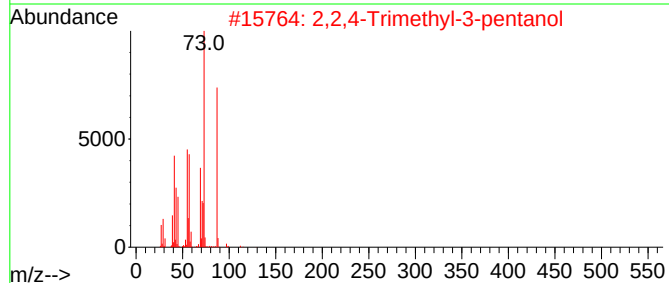
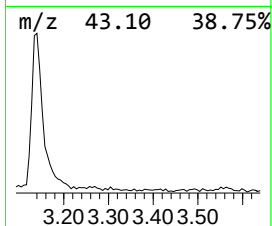
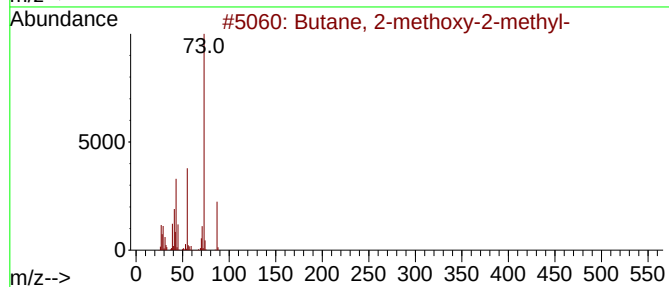
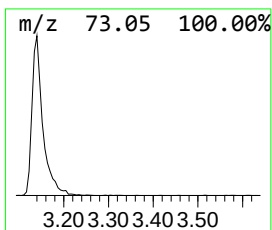
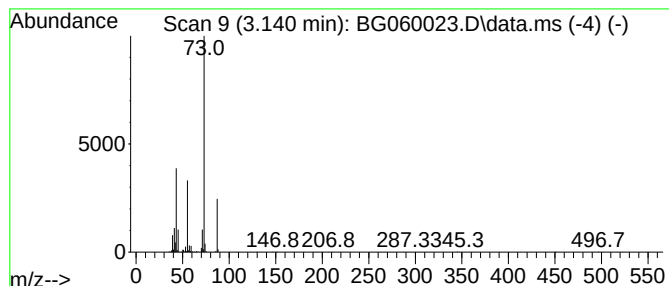
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	31.02 ng	996245	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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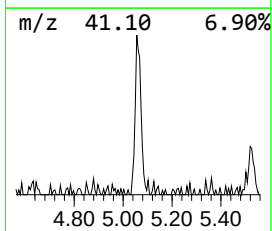
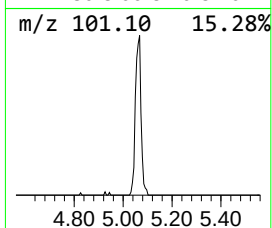
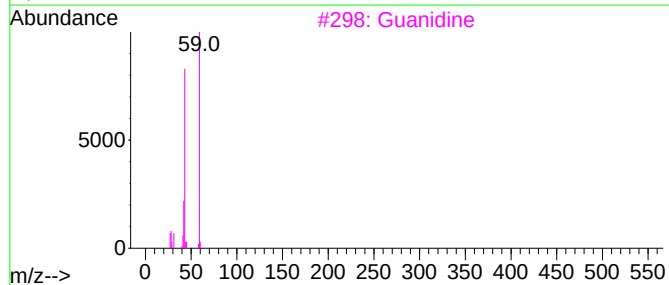
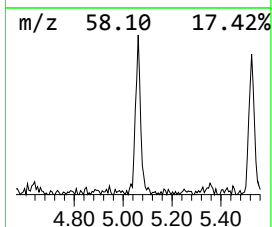
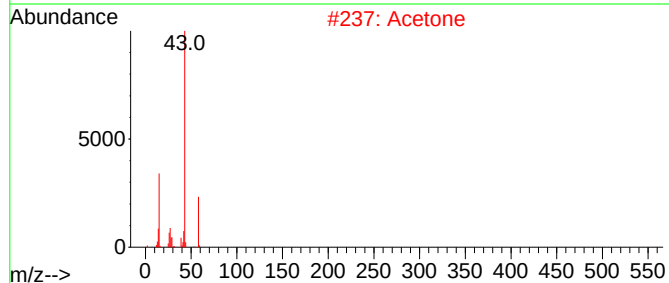
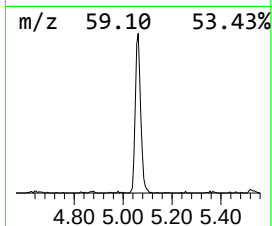
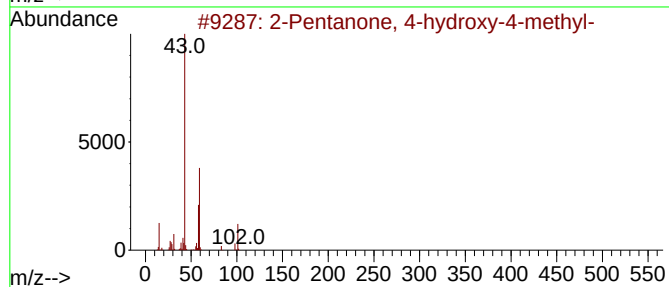
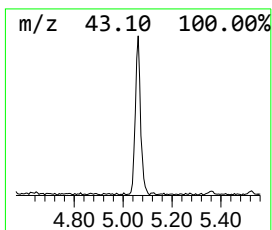
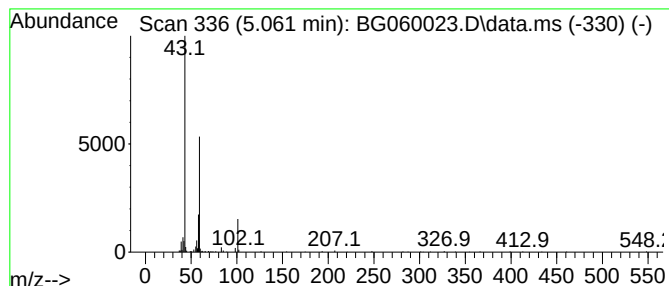
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.061	9.16 ng	294345	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetone	58	C3H6O	000067-64-1	10
3			Guanidine	59	CH5N3	000113-00-8	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7N02	016504-58-8	9
5			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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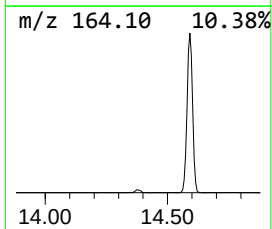
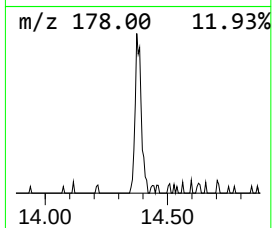
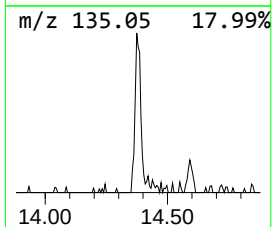
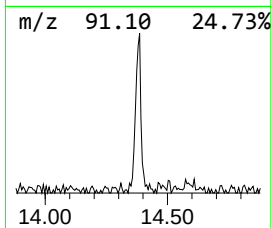
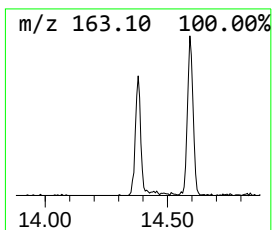
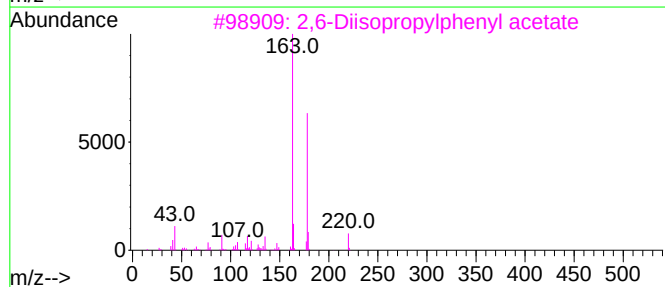
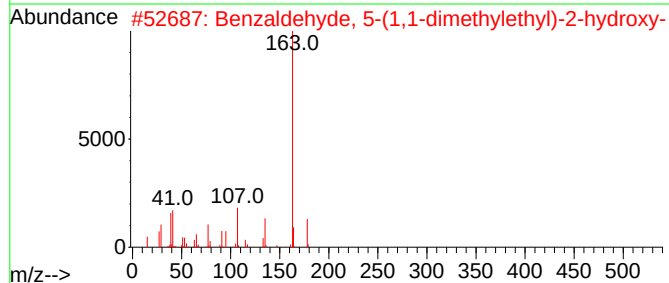
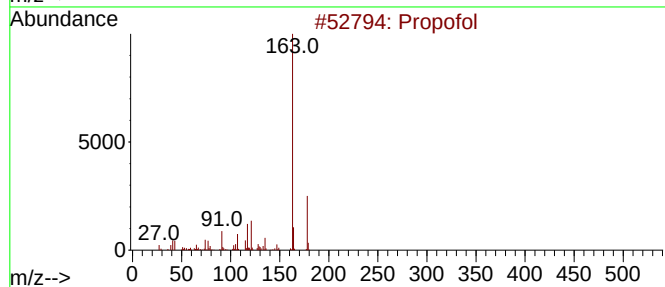
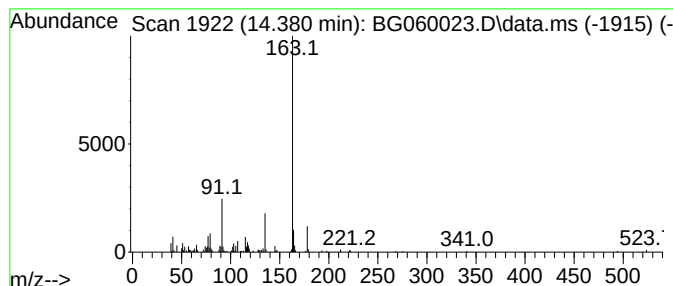
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Peak Number 3 Propofol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.380	2.28 ng	158354	Acenaphthene-d10	14.591

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propofol	178	C12H18O	002078-54-8	72
2		Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	72
3		2,6-Diisopropylphenyl acetate	220	C14H20O2	028000-66-0	64
4		2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	64
5		Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	64



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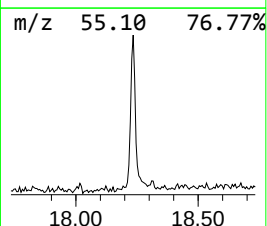
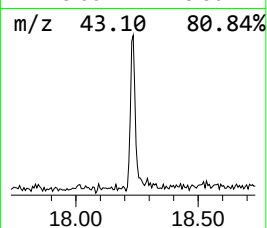
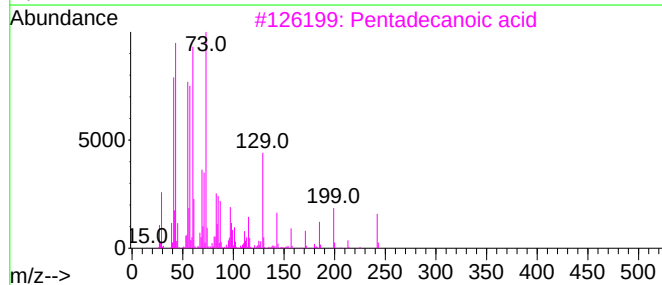
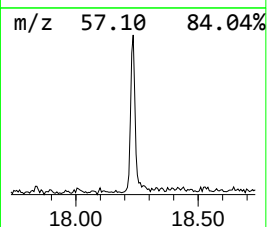
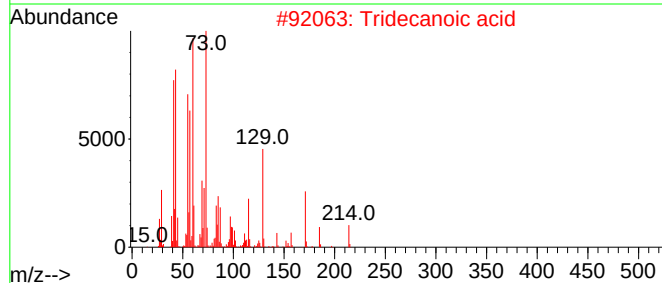
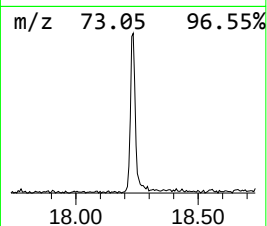
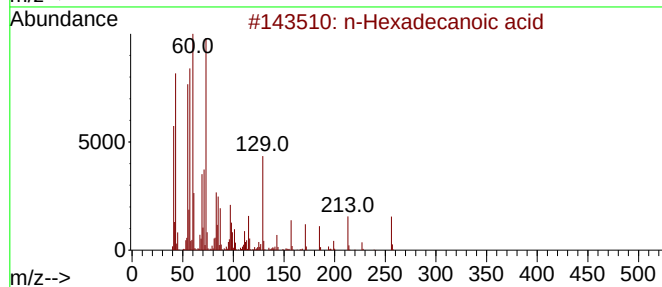
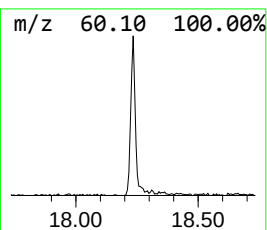
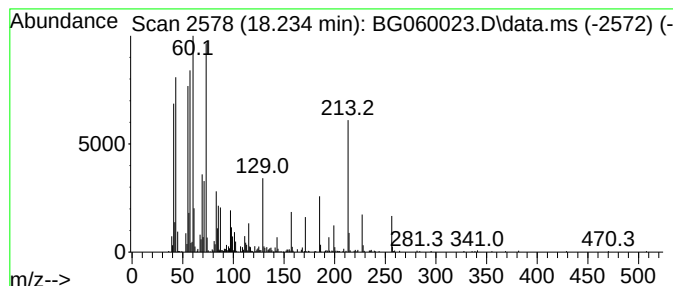
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.234	7.37 ng	689173	Phenanthrene-d10	17.341

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Octadecanoic acid	284	C18H36O2	000057-11-4	64



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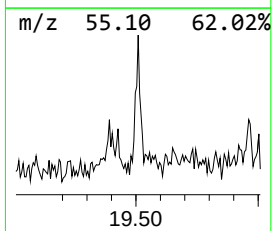
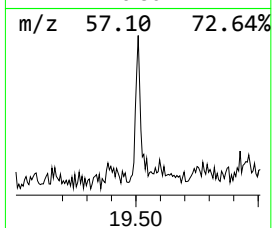
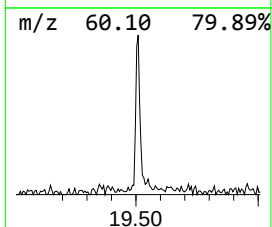
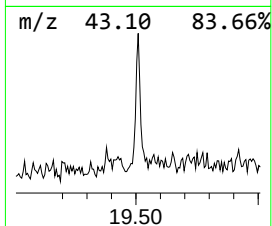
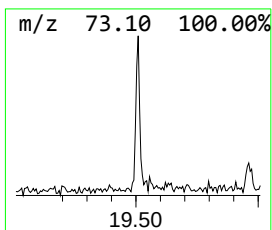
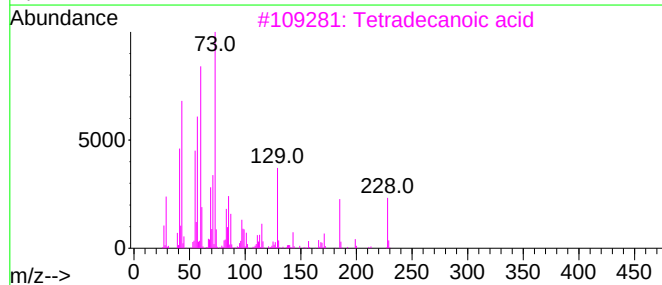
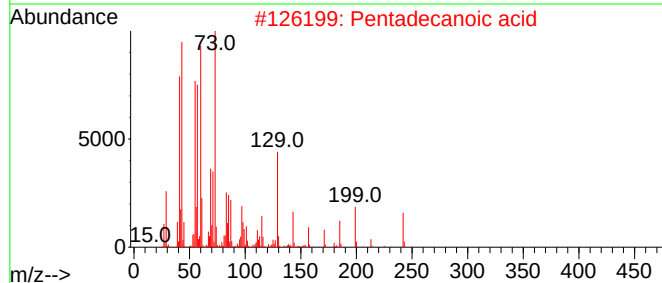
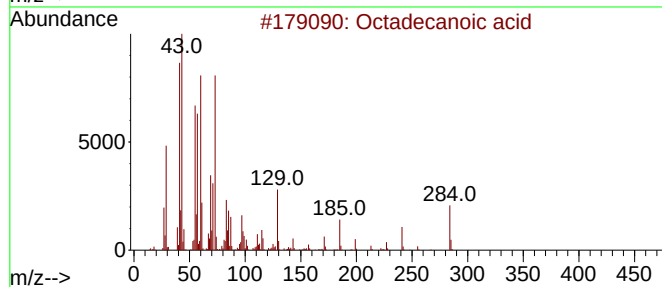
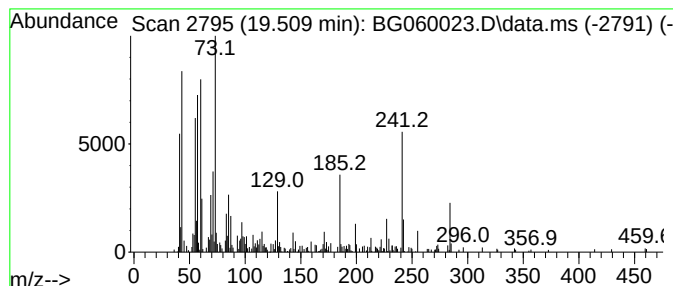
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	2.02 ng	202354	Chrysene-d12	21.607

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
5			Tridecanoic acid	214	C13H26O2	000638-53-9	49



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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
Butane, 2-metho...	3.140	31.0	ng	996245	1	7.952	642419	20.0
2-Pentanone, 4-...	5.061	9.2	ng	294345	1	7.952	642419	20.0
Propofol	14.380	2.3	ng	158354	3	14.591	1387490	20.0
n-Hexadecanoic ...	18.234	7.4	ng	689173	4	17.341	1869200	20.0
Octadecanoic acid	19.509	2.0	ng	202354	5	21.607	1999990	20.0