

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
 Data File : BM042424.D
 Acq On : 24 Oct 2023 17:53
 Operator : MA/JU
 Sample : 04960-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 VAUX-SLUDGE

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-BM102123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.445	209	214	227	rVB	1576190	2008315	30.99%	5.001%
2	5.075	315	321	332	rVB	2499946	3315584	51.16%	8.256%
3	5.522	391	397	410	rBV	2720405	3899360	60.16%	9.710%
4	6.157	499	505	512	rBV	91064	133327	2.06%	0.332%
5	7.145	666	673	685	rBV	2611603	4013474	61.92%	9.994%
6	7.992	811	817	829	rBV	557662	880231	13.58%	2.192%
7	9.192	1013	1021	1035	rBV	1539091	2461904	37.98%	6.130%
8	10.816	1289	1297	1305	rBV	713219	1169464	18.04%	2.912%
9	13.263	1706	1713	1727	rBV	3220976	4657209	71.85%	11.597%
10	14.639	1941	1947	1957	rVB	949173	1341956	20.70%	3.342%
11	16.133	2192	2201	2211	rBV	2433055	3391674	52.33%	8.445%
12	17.392	2408	2415	2421	rBV	1129737	1551954	23.94%	3.864%
13	18.239	2554	2559	2569	rBV	359566	592044	9.13%	1.474%
14	19.515	2771	2776	2784	rBV	234135	366401	5.65%	0.912%
15	20.003	2853	2859	2869	rBV	5523691	6481403	100.00%	16.139%
16	21.233	3064	3068	3074	rBV6	58789	104535	1.61%	0.260%
17	21.574	3121	3126	3134	rBV	1432263	1783227	27.51%	4.440%
18	24.038	3538	3545	3561	rVB	933014	2007573	30.97%	4.999%

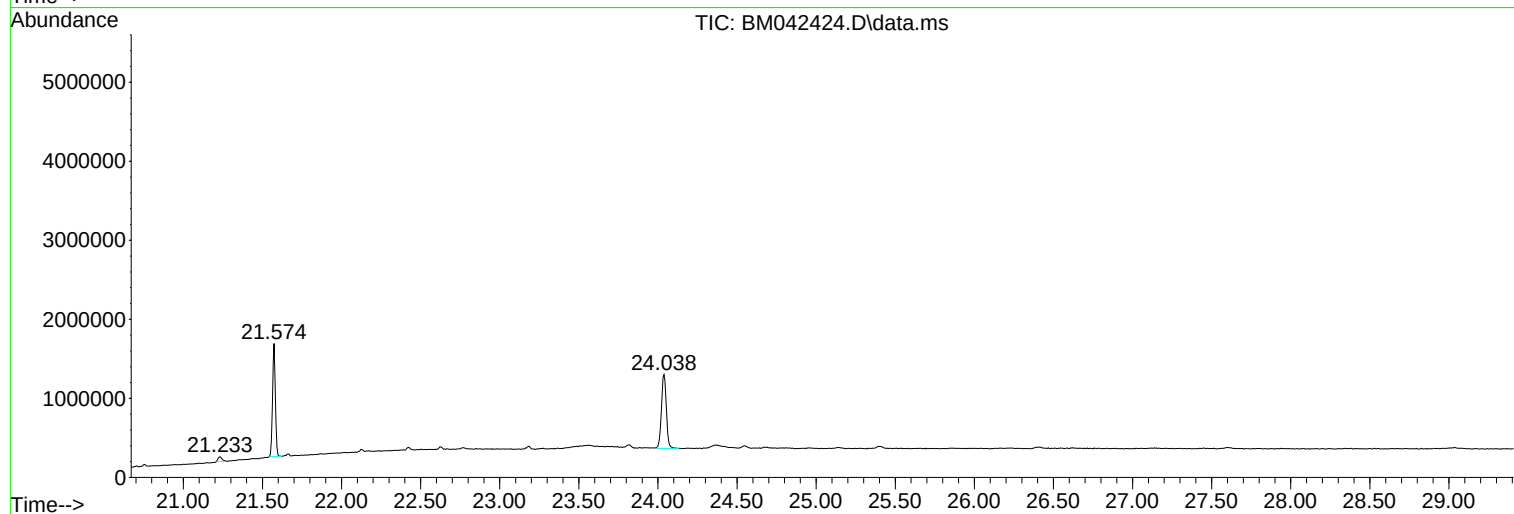
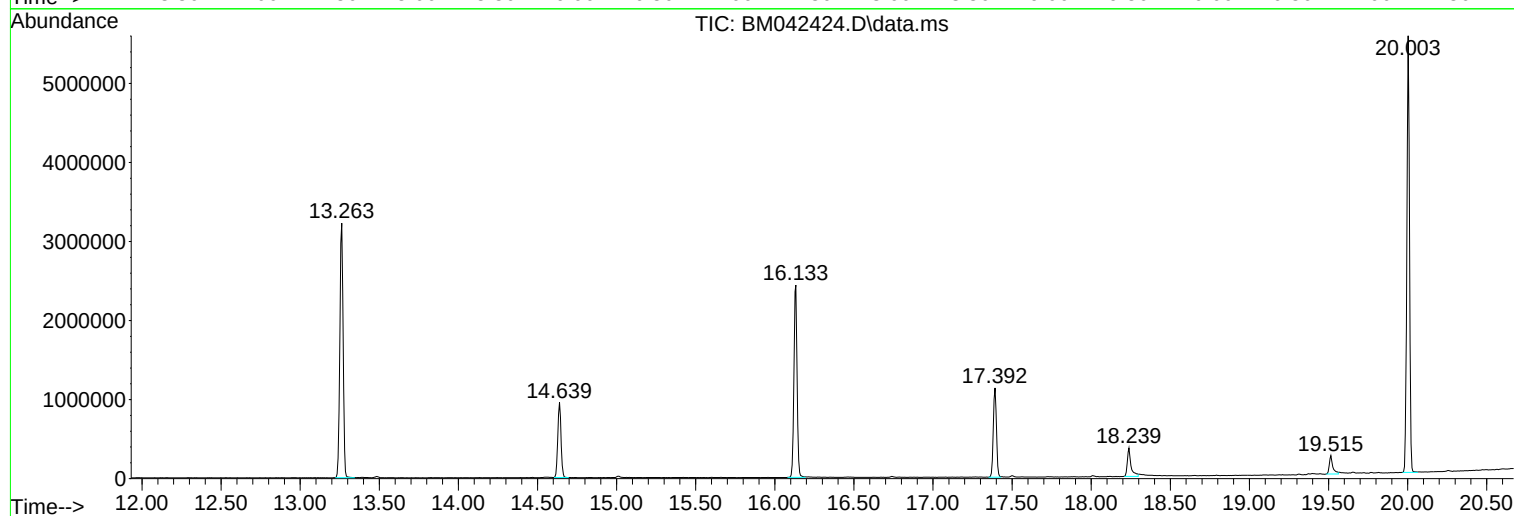
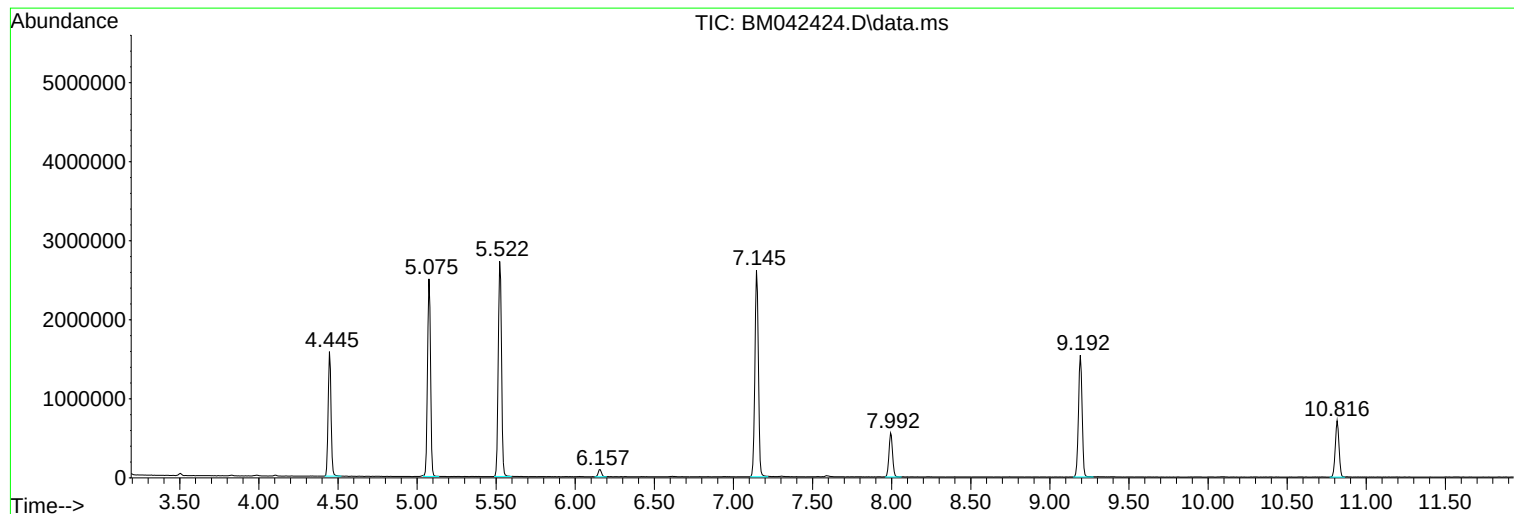
Sum of corrected areas: 40159635

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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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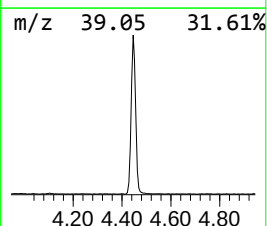
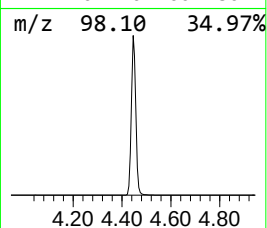
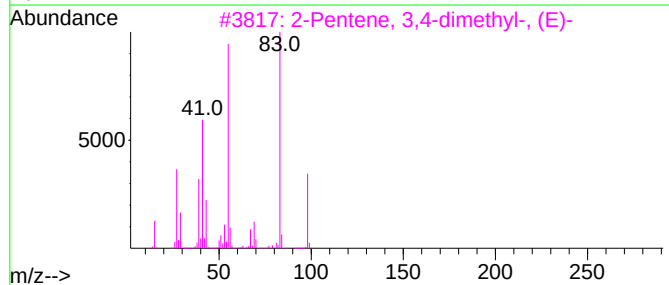
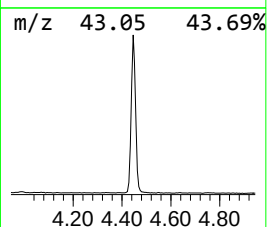
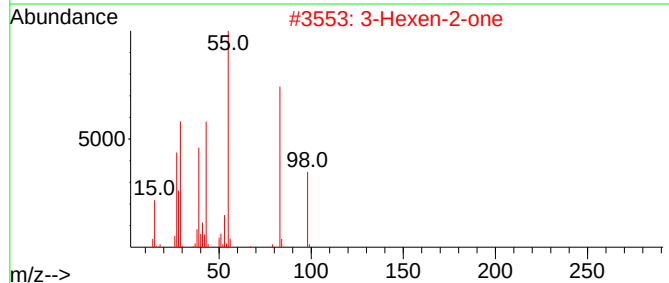
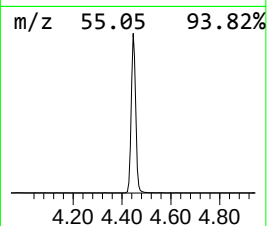
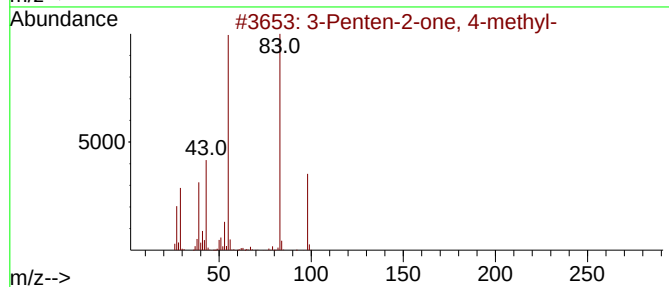
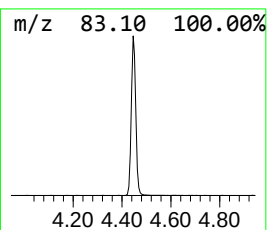
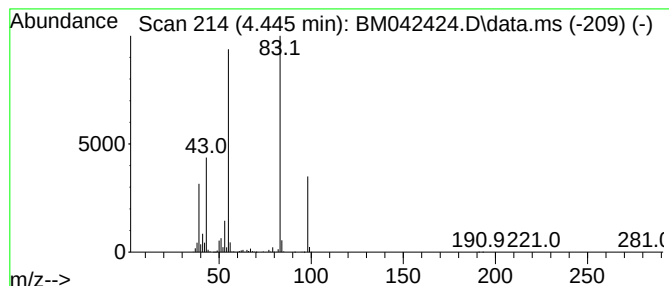
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.445	45.63 ng	2008320	1,4-Dichlorobenzene-d4	7.992

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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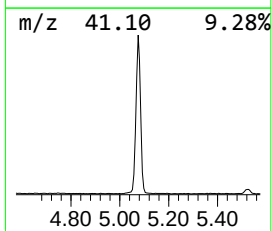
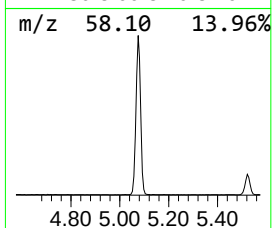
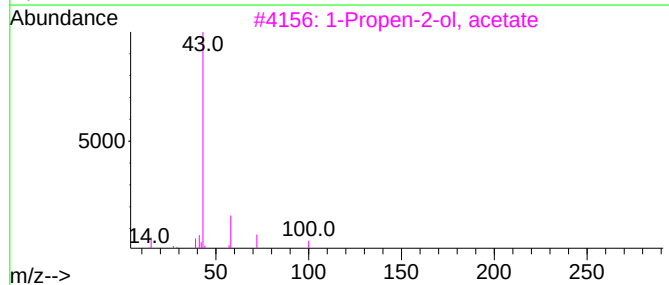
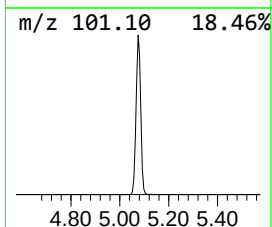
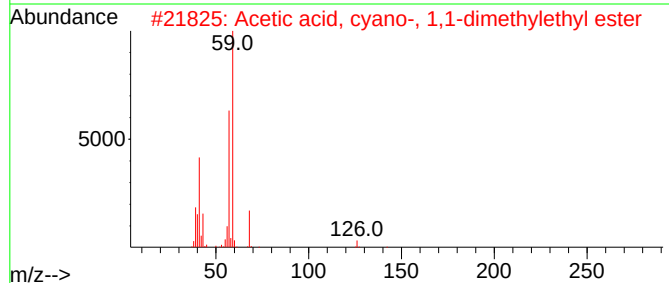
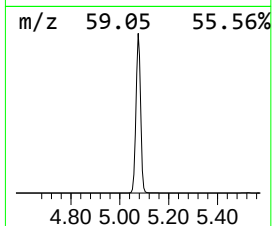
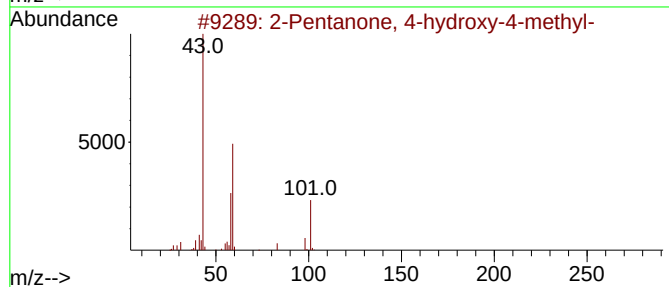
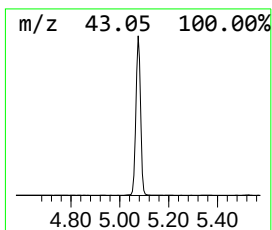
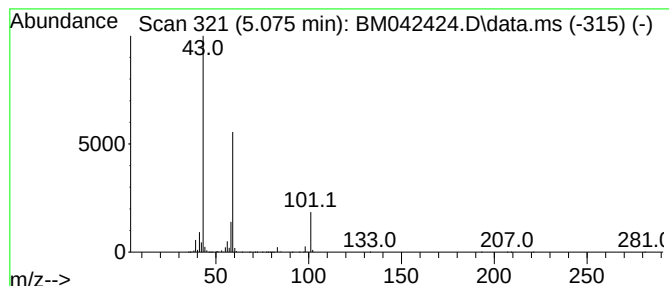
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	75.33 ng	3315580	1,4-Dichlorobenzene-d4	7.992

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	32
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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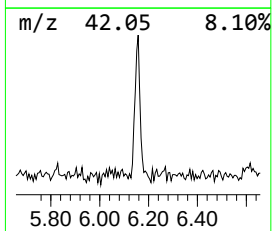
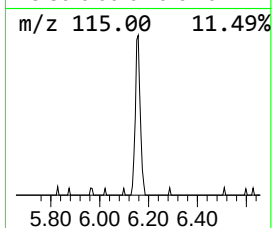
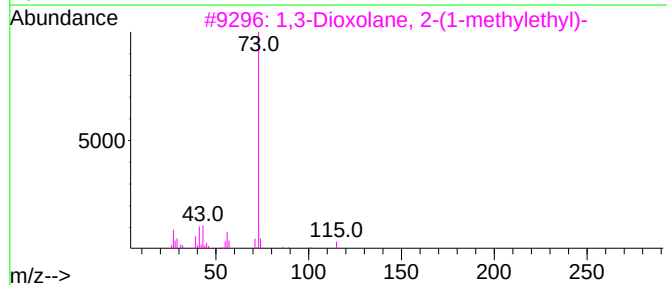
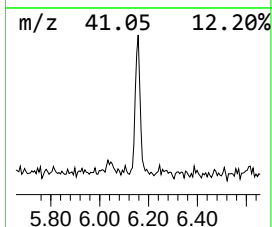
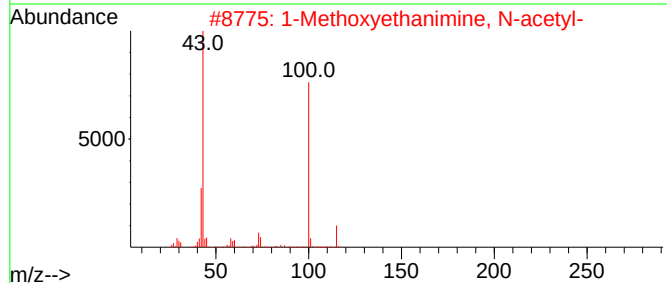
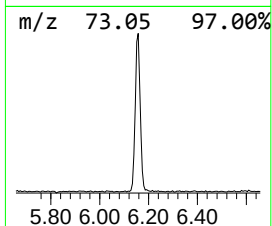
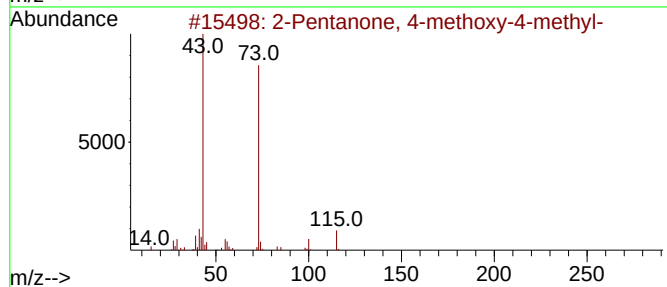
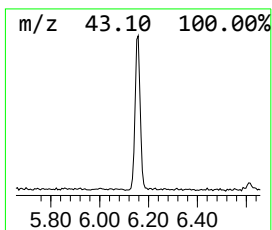
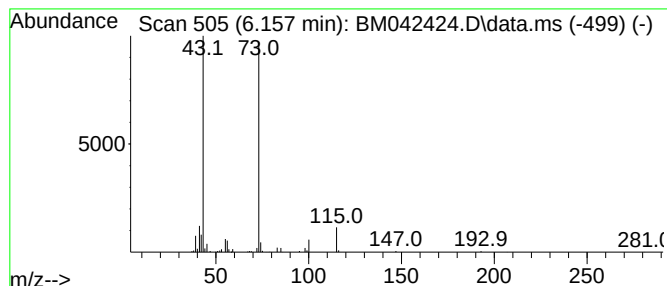
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.157	3.03 ng	133327	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	38
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4			N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5			6-Hydroxy-4,4,6-trimethyltetrahy...	191	C7H13NO5	016504-29-3	10



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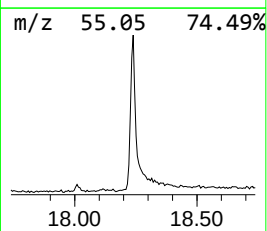
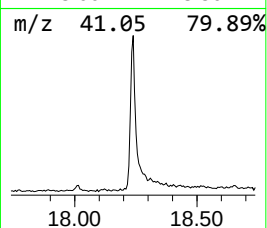
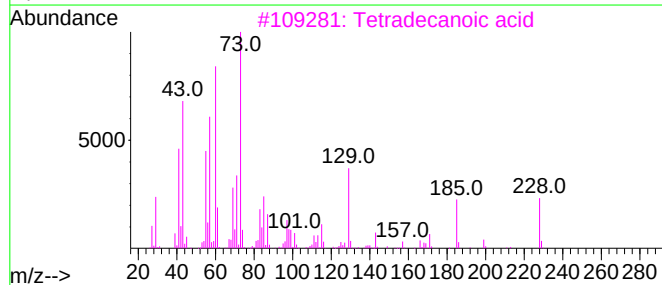
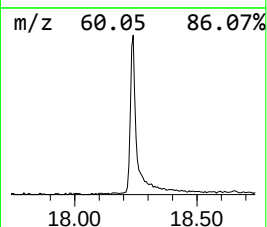
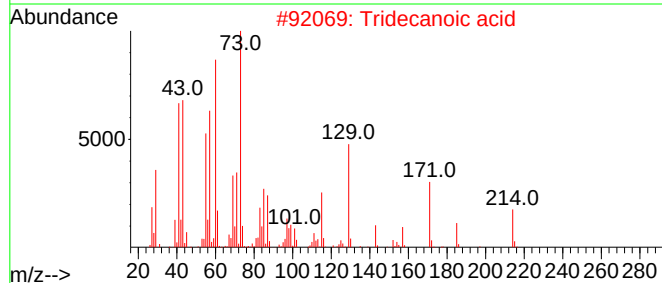
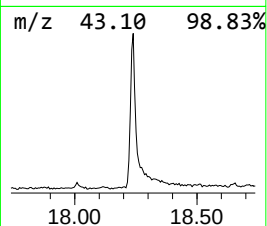
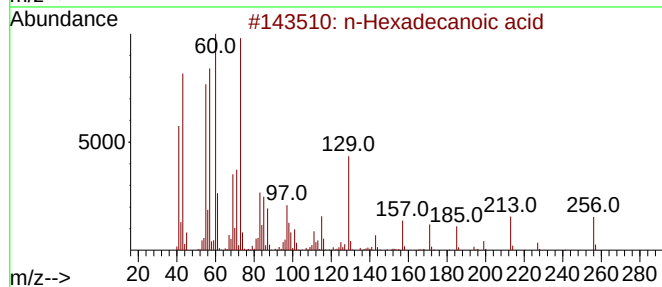
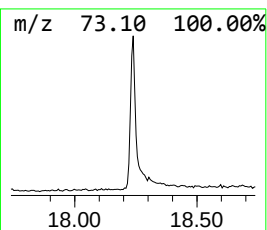
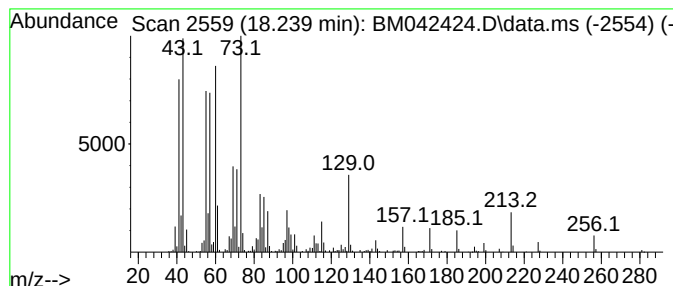
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	7.63 ng	592044	Phenanthrene-d10	17.392

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	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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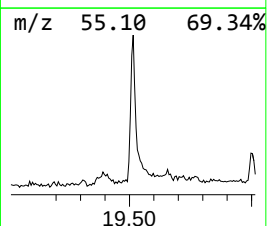
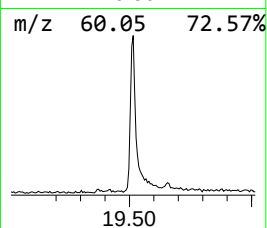
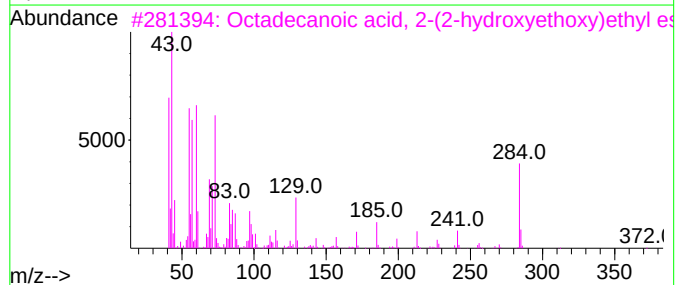
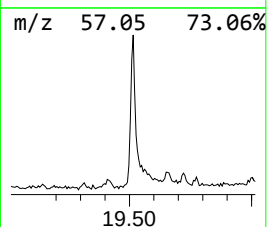
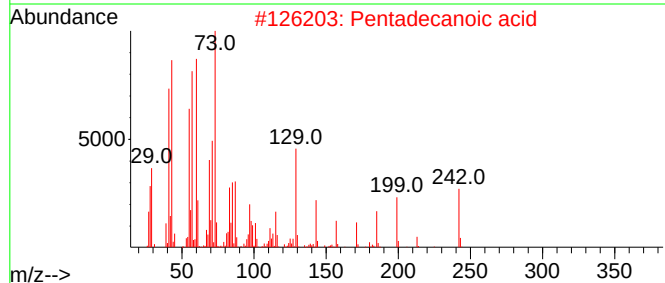
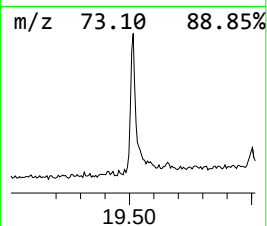
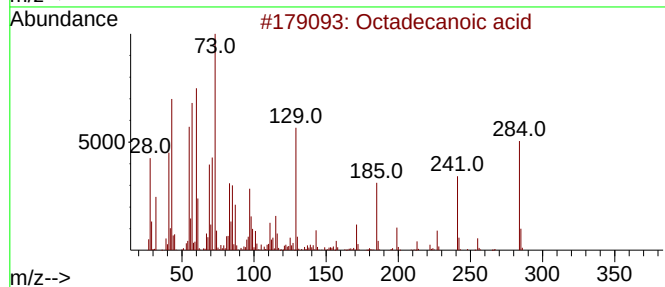
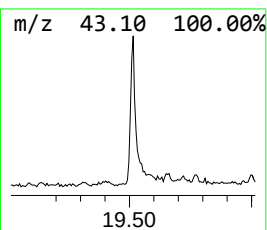
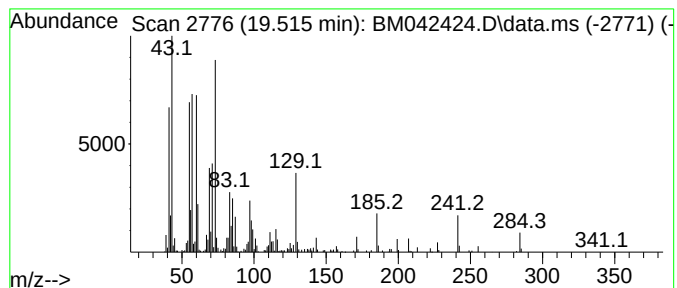
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	4.11 ng	366401	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.445	45.6	ng	2008320	1	7.992	880231	20.0
2-Pentanone, 4-...	5.075	75.3	ng	3315580	1	7.992	880231	20.0
2-Pentanone, 4-...	6.157	3.0	ng	133327	1	7.992	880231	20.0
n-Hexadecanoic ...	18.239	7.6	ng	592044	4	17.392	1551950	20.0
Octadecanoic acid	19.515	4.1	ng	366401	5	21.574	1783230	20.0