

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
 Data File : BG055832.D
 Acq On : 29 Nov 2022 17:23
 Operator : CG/JU
 Sample : N5796-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-N

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.276	330	338	351	rBV	294107	464752	27.06%	4.459%
2	5.757	413	420	436	rVB	450134	745065	43.37%	7.149%
3	6.374	518	525	532	rBV	18280	30234	1.76%	0.290%
4	7.373	687	695	710	rBV	458380	811547	47.25%	7.787%
5	8.225	833	840	847	rBV	154420	263519	15.34%	2.529%
6	9.394	1030	1039	1049	rBV	286971	510891	29.74%	4.902%
7	10.799	1270	1278	1299	rBV2	42553	129336	7.53%	1.241%
8	11.051	1314	1321	1329	rBV	220232	383700	22.34%	3.682%
9	13.472	1724	1733	1742	rBV	819406	1241430	72.27%	11.912%
10	14.847	1960	1967	1975	rVB	367147	555798	32.36%	5.333%
11	16.186	2189	2195	2204	rVB	25324	39477	2.30%	0.379%
12	16.327	2213	2219	2229	rBV	630215	980418	57.08%	9.407%
13	17.585	2427	2433	2439	rBV	424316	672293	39.14%	6.451%
14	18.219	2537	2541	2545	rBV	21808	28410	1.65%	0.273%
15	18.448	2575	2580	2587	rBV2	51948	106194	6.18%	1.019%
16	18.654	2609	2615	2618	rBV4	18125	40841	2.38%	0.392%
17	18.860	2646	2650	2653	rBV3	30537	36279	2.11%	0.348%
18	19.377	2730	2738	2742	rBV2	41712	95197	5.54%	0.913%
19	19.624	2777	2780	2785	rVB	29323	42686	2.49%	0.410%
20	19.706	2792	2794	2798	rBV4	17223	21747	1.27%	0.209%
21	19.988	2838	2842	2848	rVB	71506	112348	6.54%	1.078%
22	20.170	2868	2873	2879	rVB	1308651	1717740	100.00%	16.482%
23	21.880	3158	3164	3170	rVB	388676	658604	38.34%	6.320%
24	25.270	3734	3741	3753	rVB2	251074	733164	42.68%	7.035%

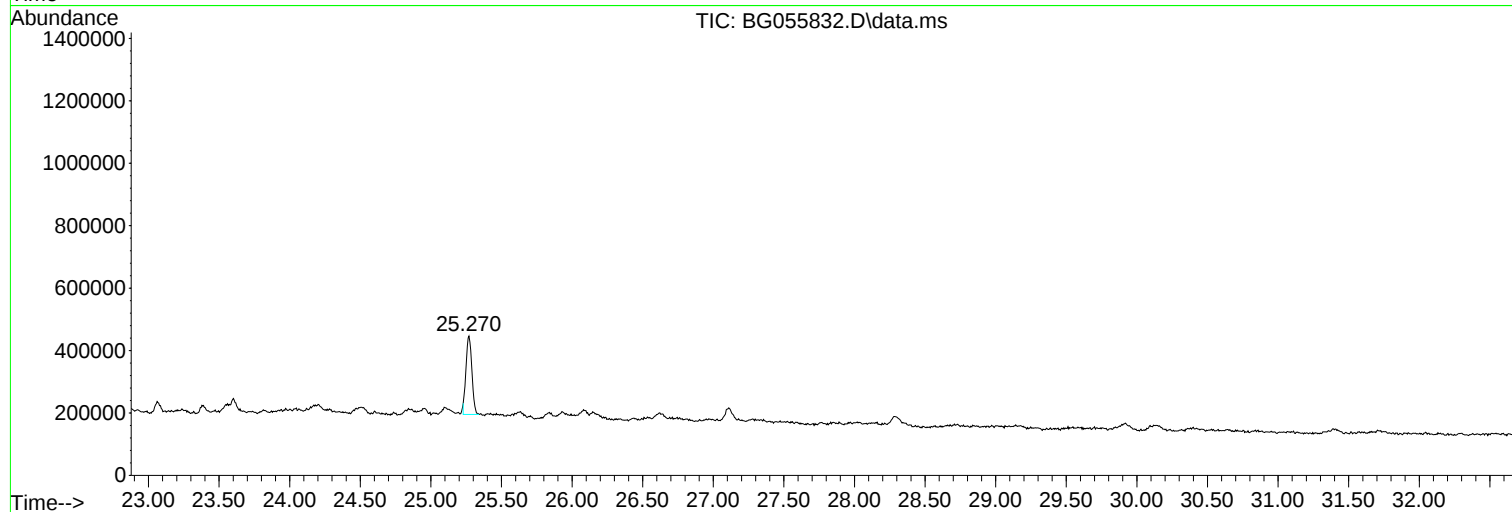
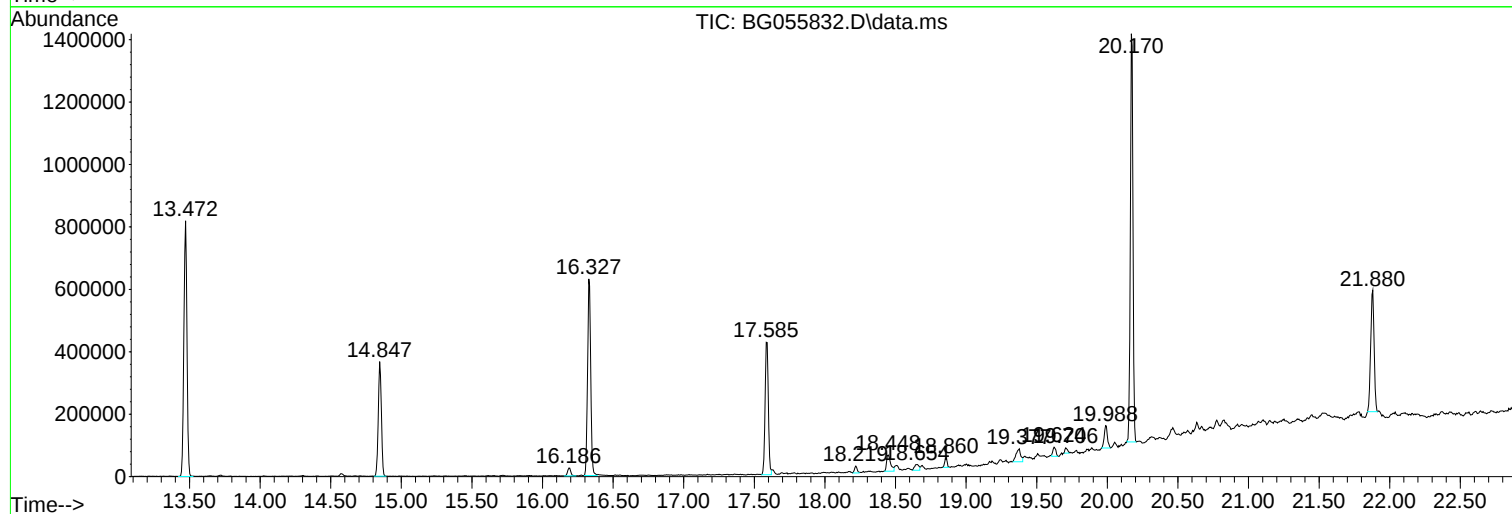
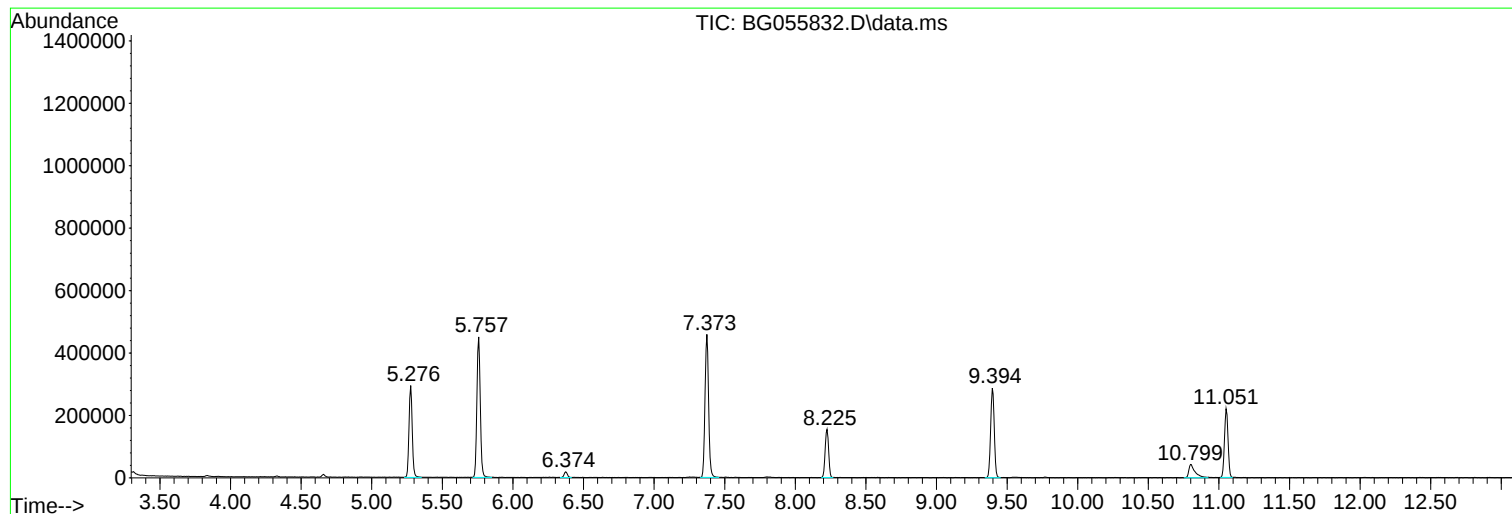
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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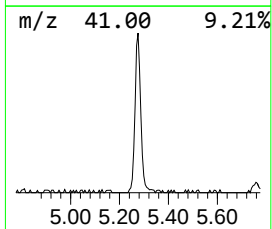
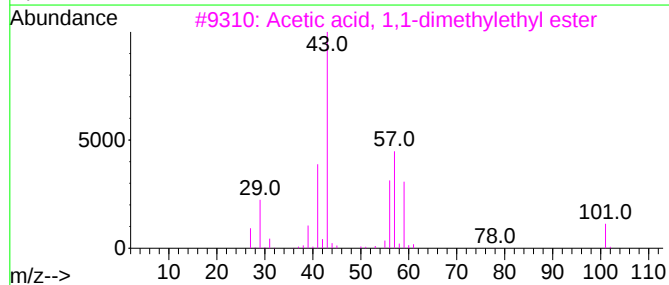
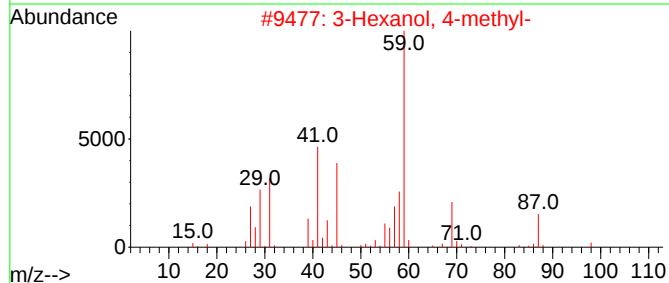
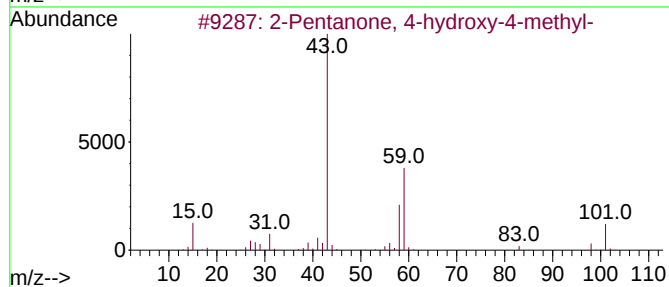
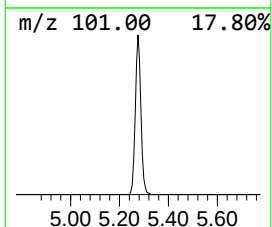
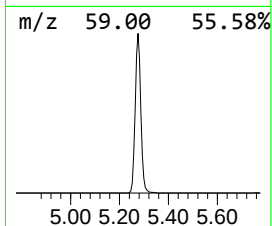
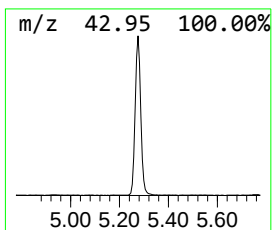
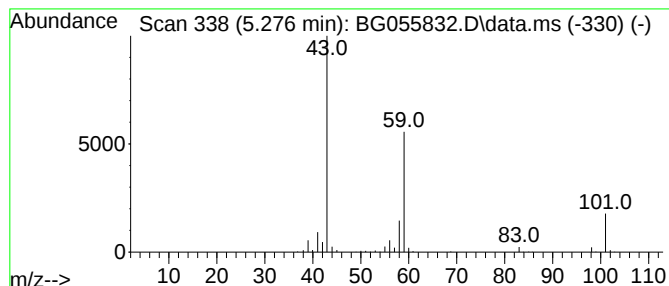
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.276	35.27 ng	464752	1,4-Dichlorobenzene-d4	8.225

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	



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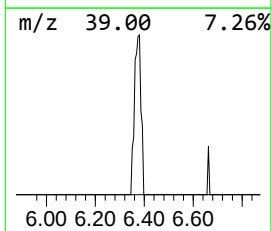
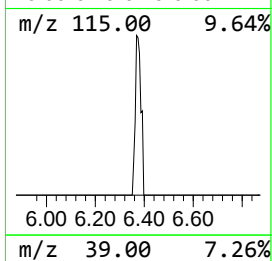
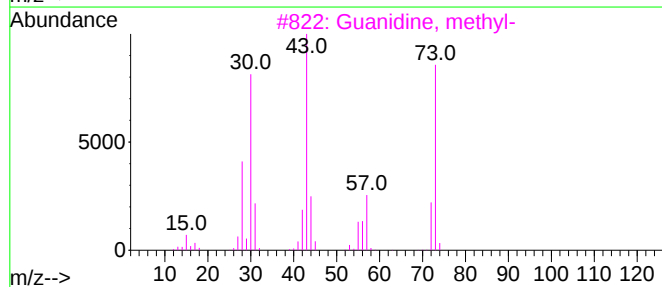
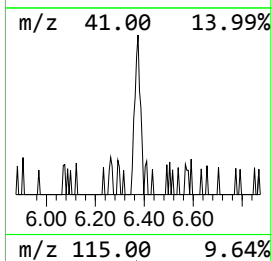
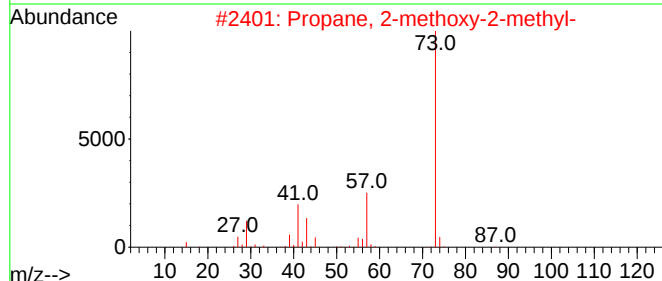
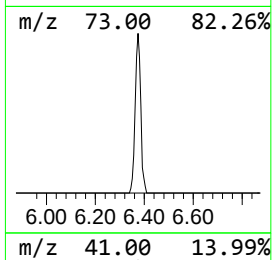
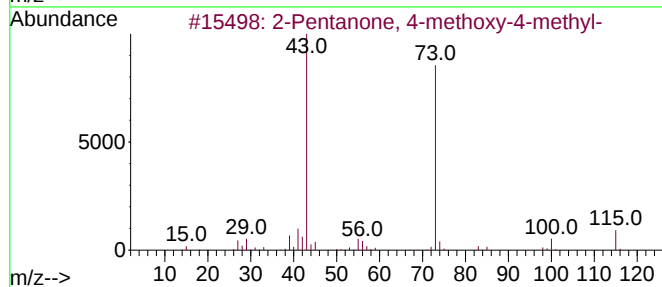
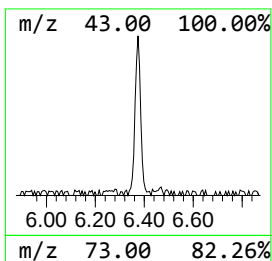
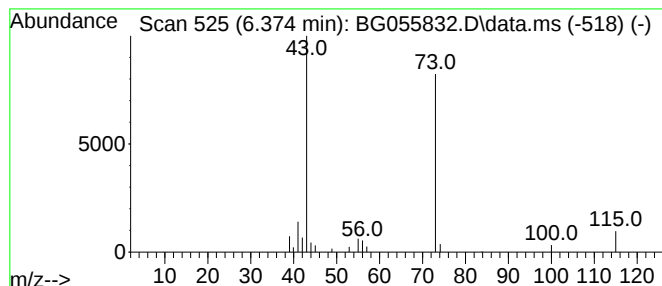
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Peak Number 2 unknown6.374 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.374	2.29 ng	30234	1,4-Dichlorobenzene-d4	8.225

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	40
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
3		Guanidine, methyl-	73	C2H7N3	000471-29-4	9
4		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
5		Di-n-propyl ether	102	C6H14O	000111-43-3	9



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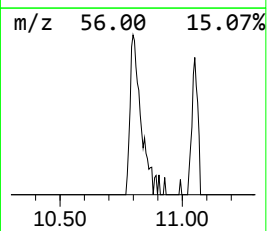
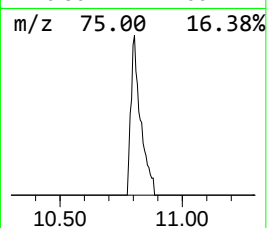
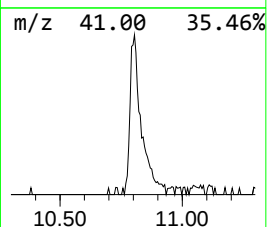
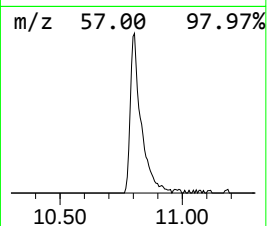
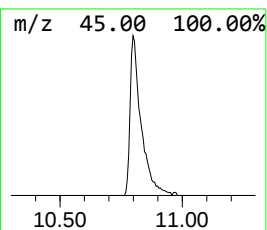
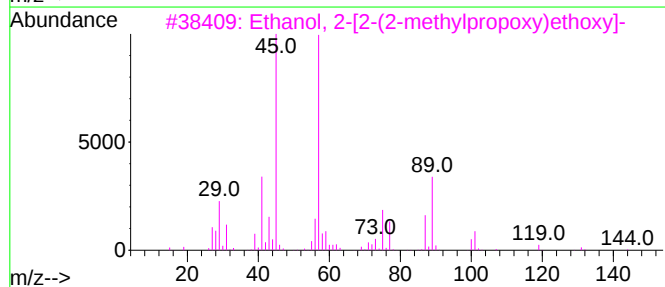
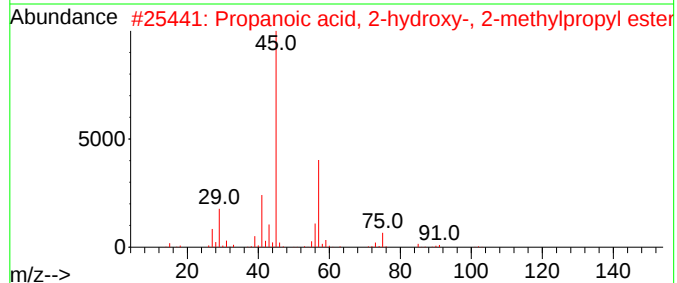
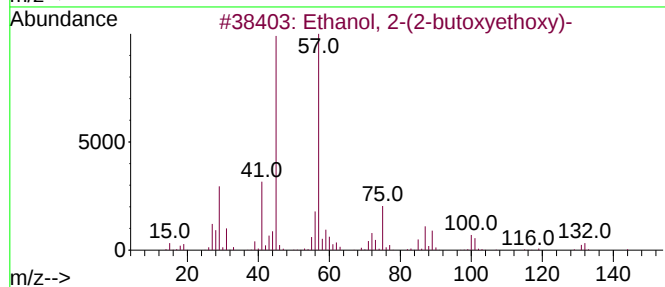
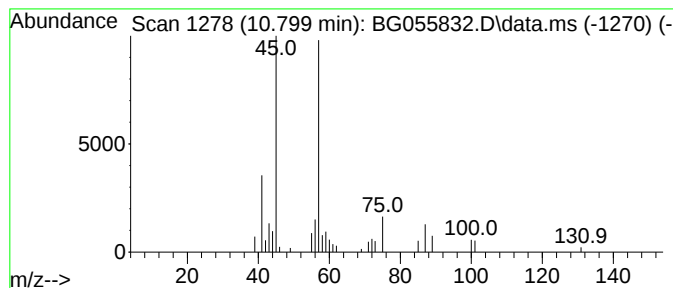
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.799	6.74 ng	129336	Naphthalene-d8	11.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



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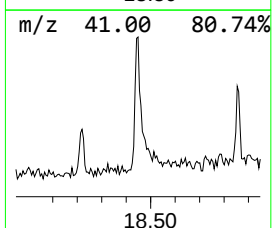
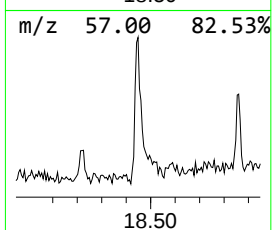
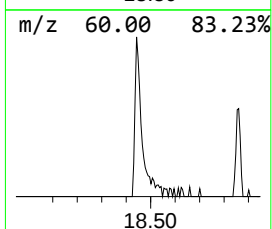
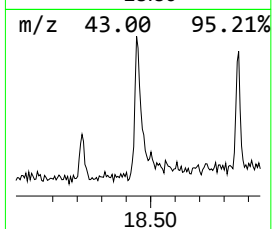
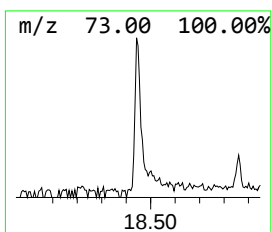
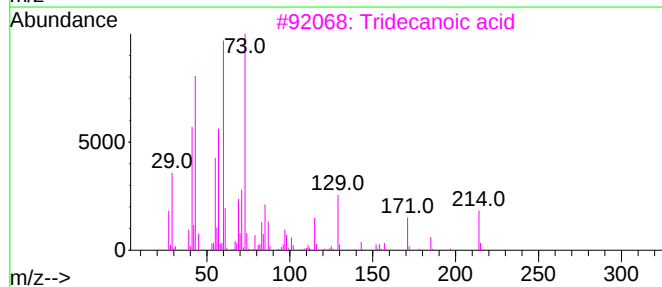
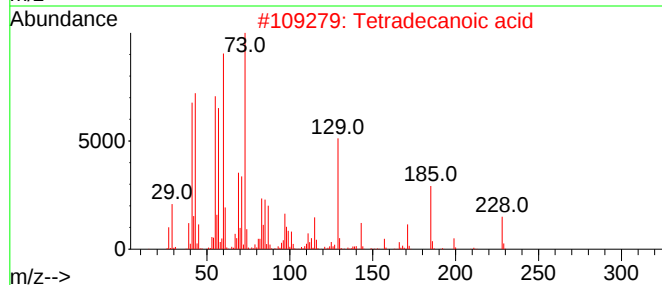
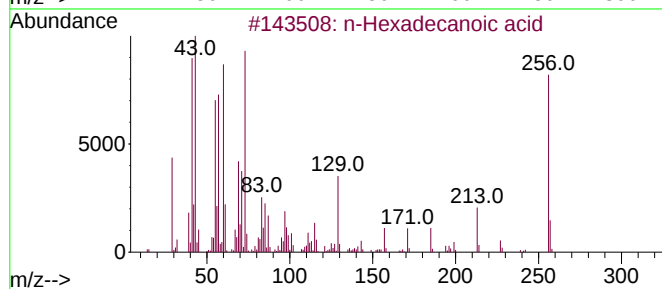
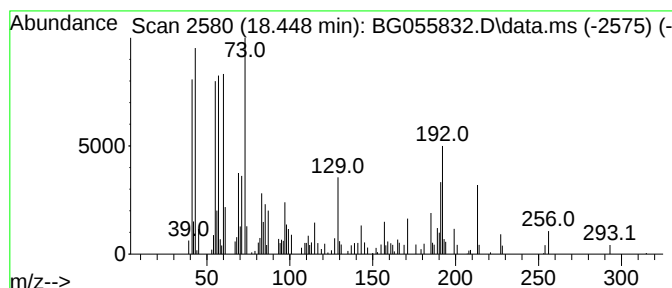
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.448	3.16 ng	106194	Phenanthrene-d10	17.591

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Octadecanoic acid	284	C18H36O2	000057-11-4	70
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	70



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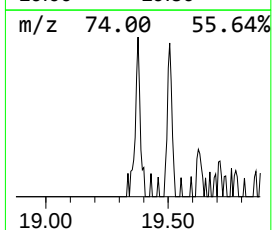
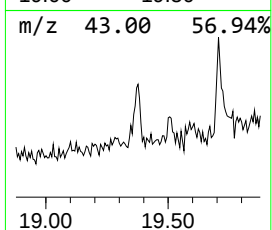
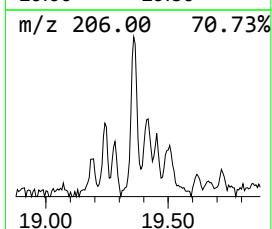
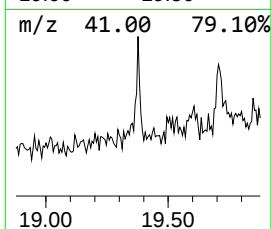
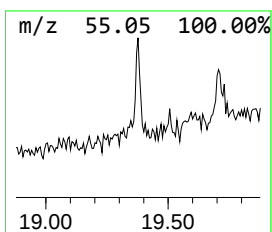
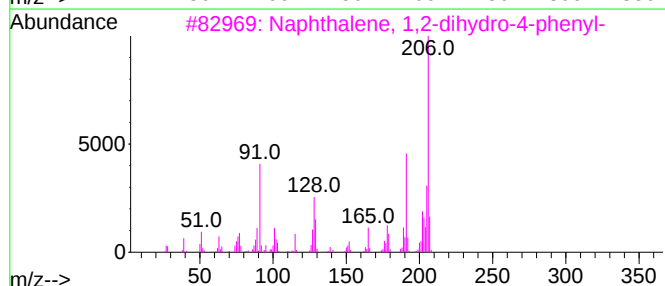
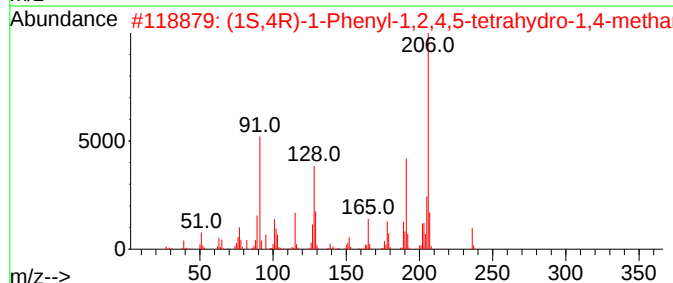
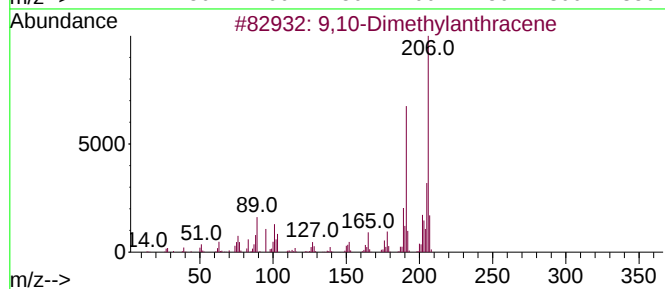
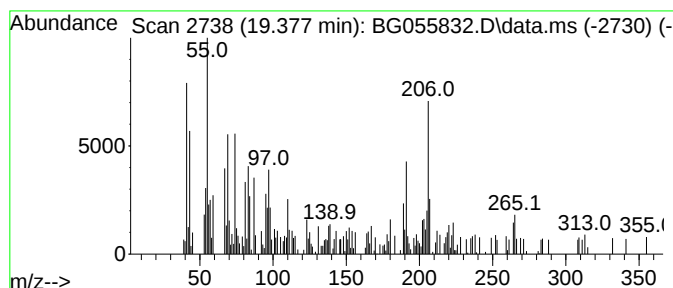
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9,10-Dimethylantracene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.377	2.83 ng	95197	Phenanthrene-d10	17.591

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,10-Dimethylantracene	206	C16H14	000781-43-1	90
2			(1S,4R)-1-Phenyl-1,2,4,5-tetrahy...	236	C17H16O	1000482-34-0	64
3			Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	50
4			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	50
5			di-p-Tolylacetylene	206	C16H14	002789-88-0	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.276	35.3	ng	464752	1	8.225	263519	20.0
unknown6.374	6.374	2.3	ng	30234	1	8.225	263519	20.0
Ethanol, 2-(2-b...	10.799	6.7	ng	129336	2	11.051	383700	20.0
n-Hexadecanoic ...	18.448	3.2	ng	106194	4	17.591	672293	20.0
9,10-Dimethylan...	19.377	2.8	ng	95197	4	17.591	672293	20.0