

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
 Data File : BP007029.D
 Acq On : 17 Sep 2021 16:47
 Operator : CG/JU
 Sample : M3774-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-CB-04-(1.5)

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_P\Methods\8270E-BP091621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	323	329	337	rBV	154161	233029	1.35%	0.303%
2	5.475	399	406	419	rBV	2423797	3603947	20.91%	4.692%
3	7.069	669	677	686	rBV	1426619	2227609	12.92%	2.900%
4	7.905	812	819	830	rBV	1067750	1772408	10.28%	2.308%
5	9.069	1003	1017	1026	rBV	3057334	5012351	29.08%	6.526%
6	10.493	1253	1259	1270	rBV	169892	321474	1.86%	0.419%
7	10.704	1288	1295	1303	rBV	1396960	2387861	13.85%	3.109%
8	13.163	1704	1713	1723	rBV	8340624	12179888	70.66%	15.857%
9	14.534	1936	1946	1954	rBV	2159681	3263129	18.93%	4.248%
10	16.022	2192	2199	2205	rBV	6016240	8598816	49.88%	11.195%
11	16.216	2224	2232	2242	rBV	2020461	3297658	19.13%	4.293%
12	17.281	2407	2413	2419	rBV	2621876	3681884	21.36%	4.793%
13	18.169	2559	2564	2587	rBV	1451907	2533534	14.70%	3.298%
14	19.398	2768	2773	2791	rBV	1027230	1635282	9.49%	2.129%
15	19.833	2842	2847	2856	rBV	13721114	17237440	100.00%	22.442%
16	21.069	3054	3057	3063	rBV2	269917	360999	2.09%	0.470%
17	21.357	3101	3106	3112	rBV	3345968	4179826	24.25%	5.442%
18	23.774	3510	3517	3526	rVB	2083753	4283134	24.85%	5.576%

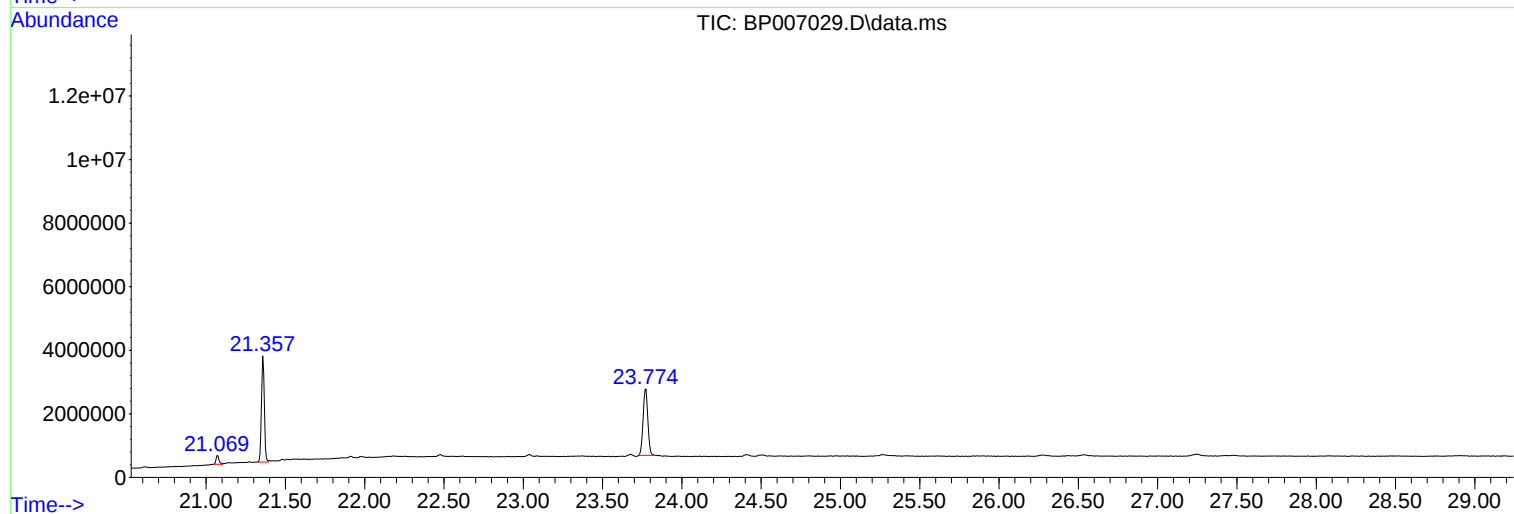
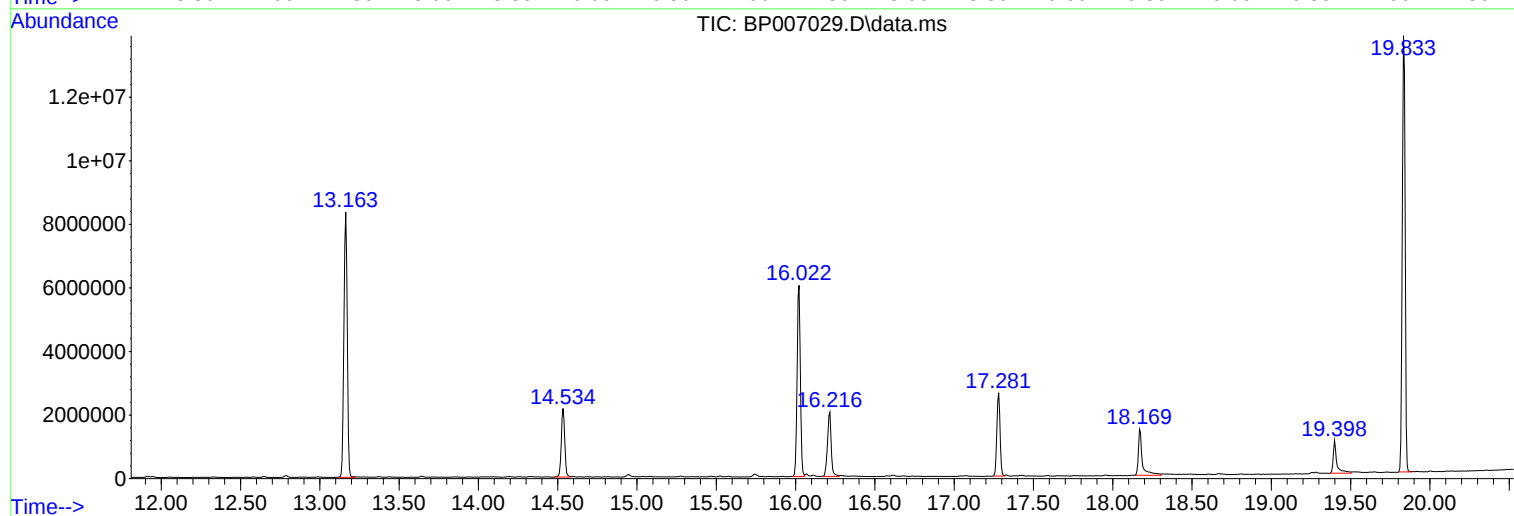
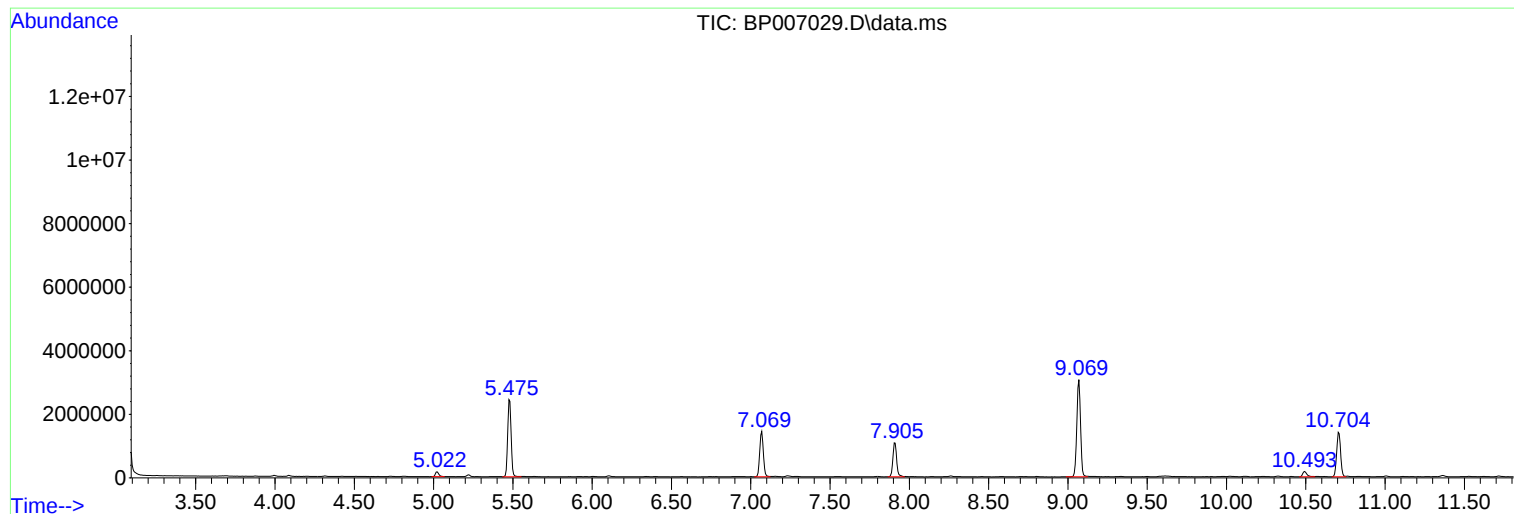
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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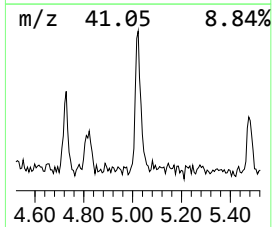
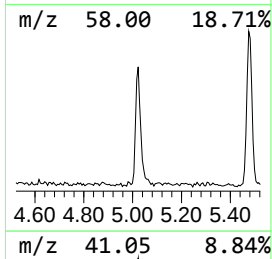
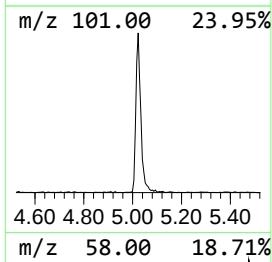
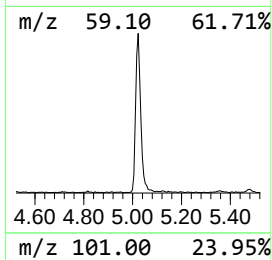
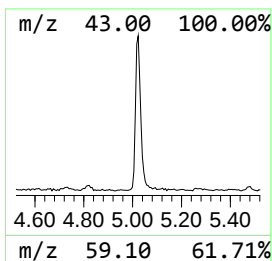
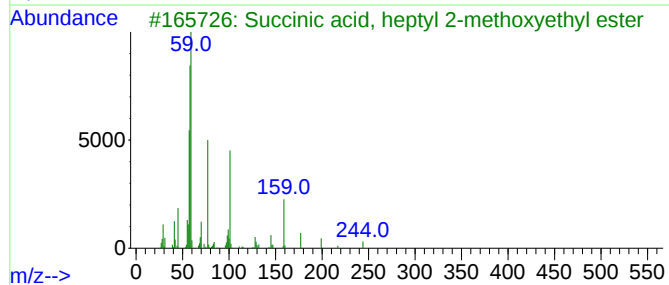
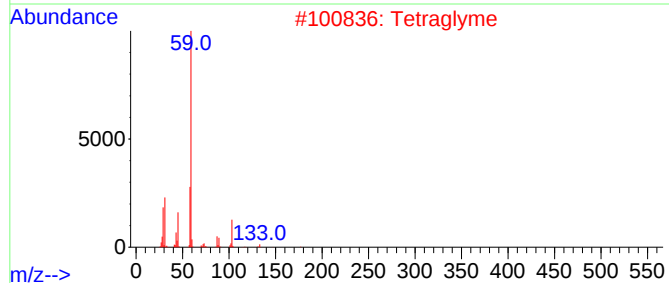
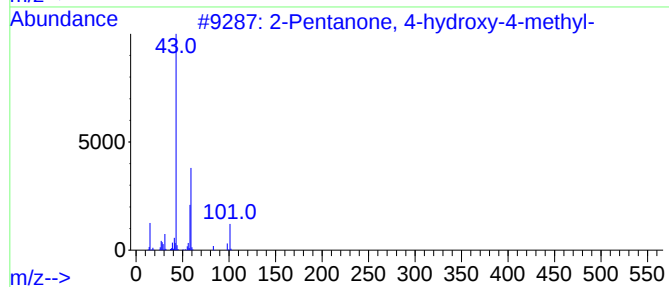
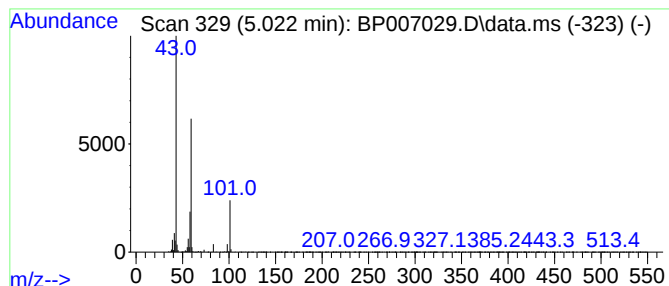
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	2.63 ng	233029	1,4-Dichlorobenzene-d4	7.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Tetraglyme	222	C10H22O5	000143-24-8	37		
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28		
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		



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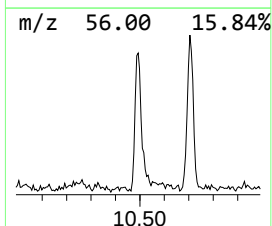
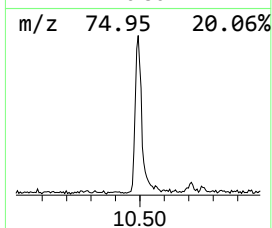
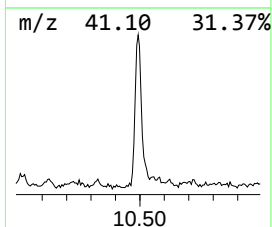
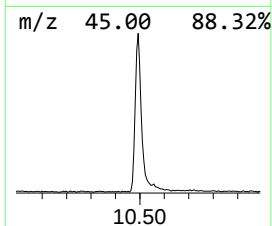
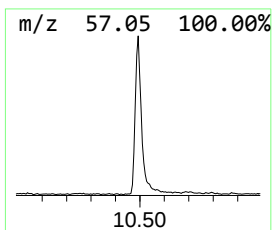
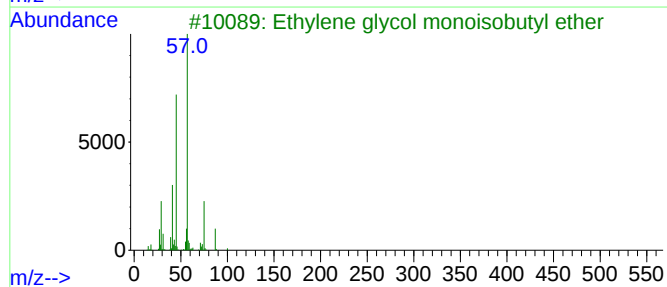
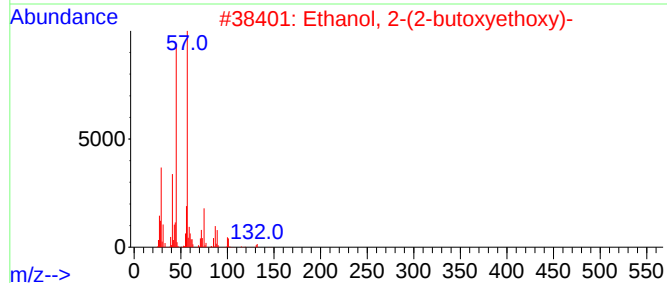
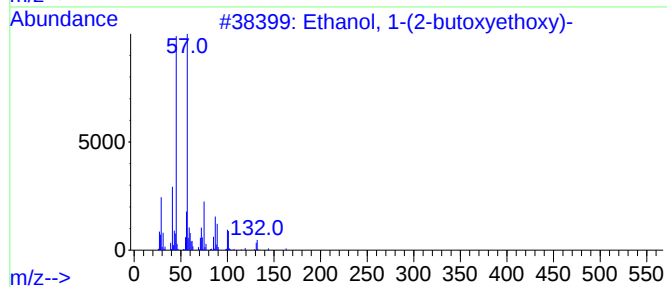
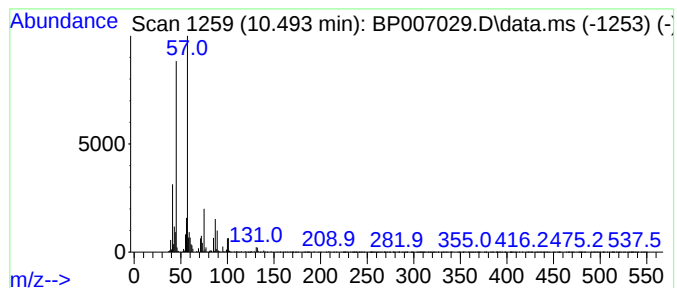
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Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.493	2.69 ng	321474	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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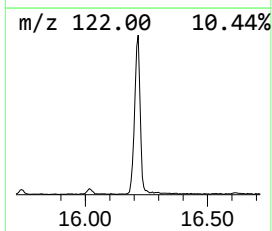
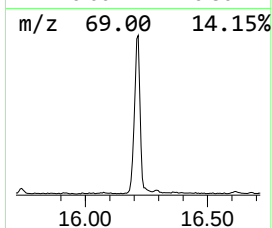
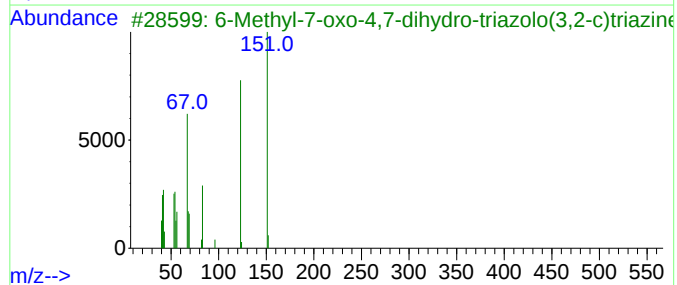
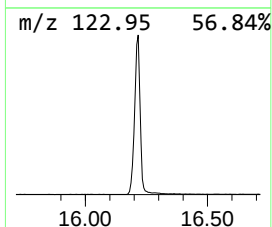
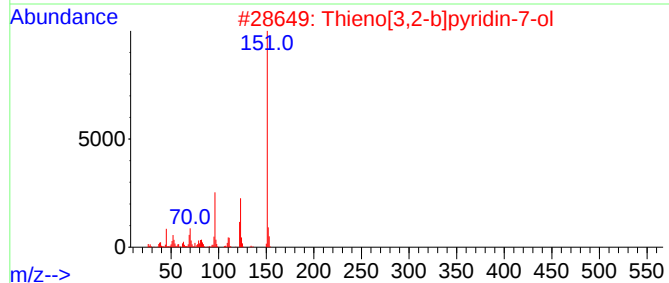
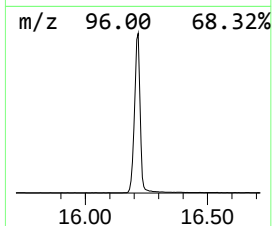
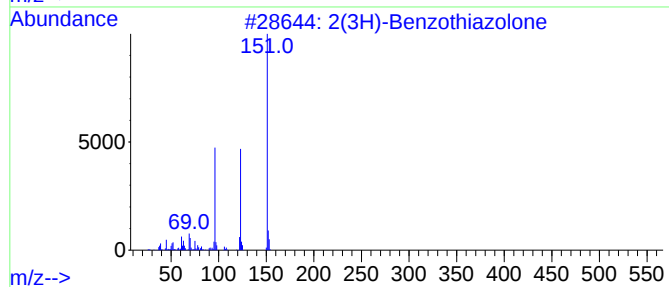
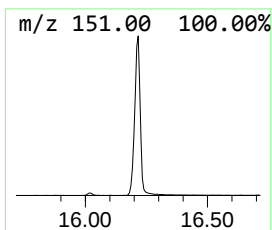
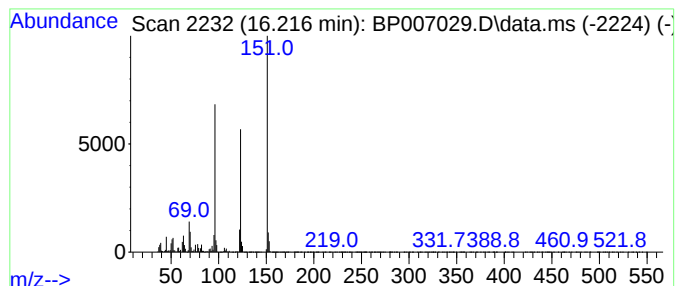
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Peak Number 3 2(3H)-Benzothiazolone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.216	17.91 ng	3297660	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
3			6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
4			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	47
5			4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	38



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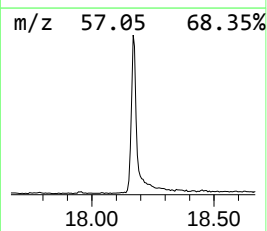
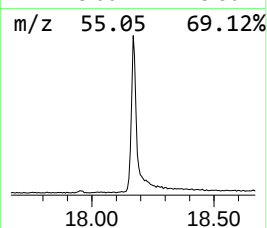
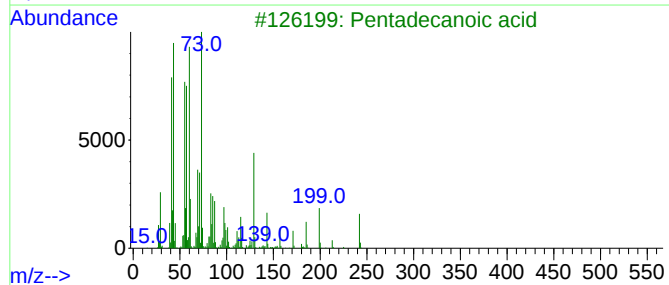
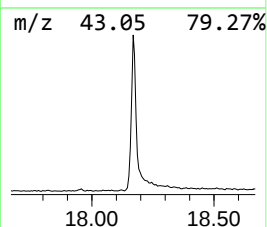
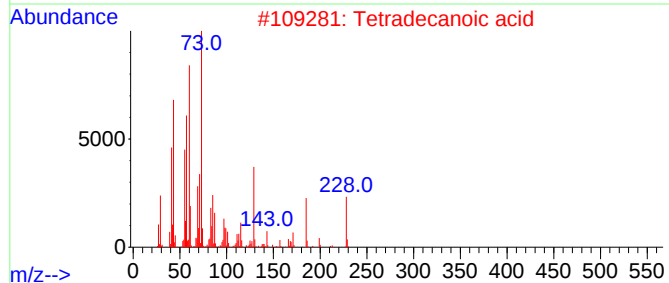
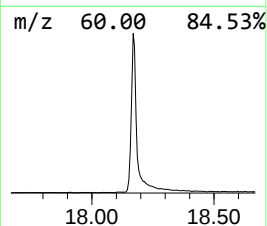
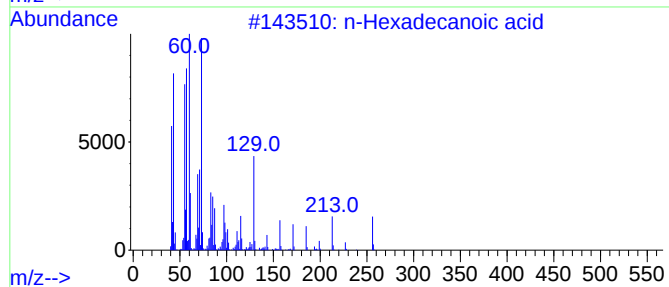
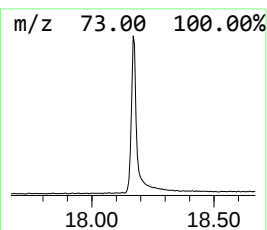
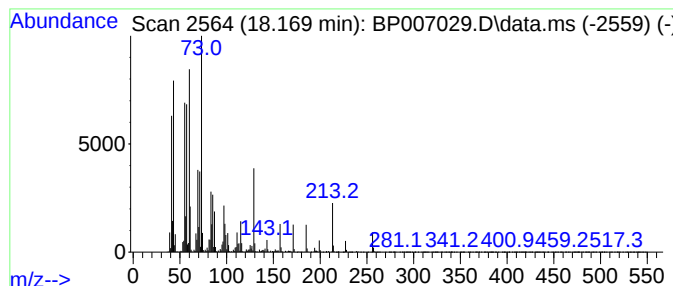
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	13.76 ng	2533530	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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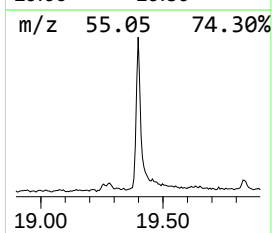
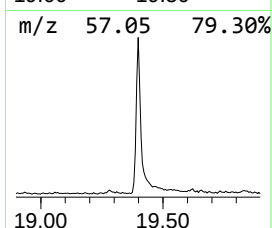
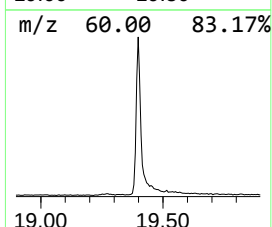
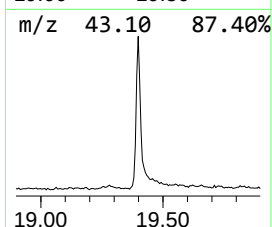
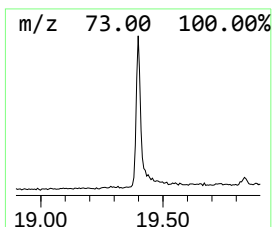
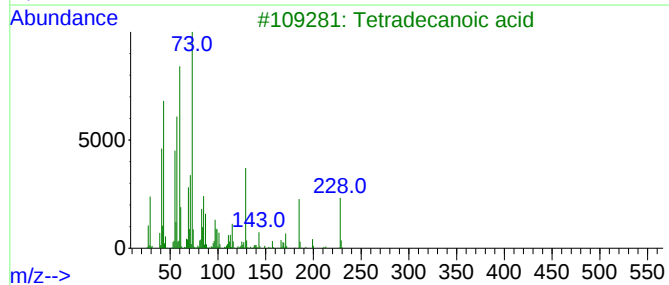
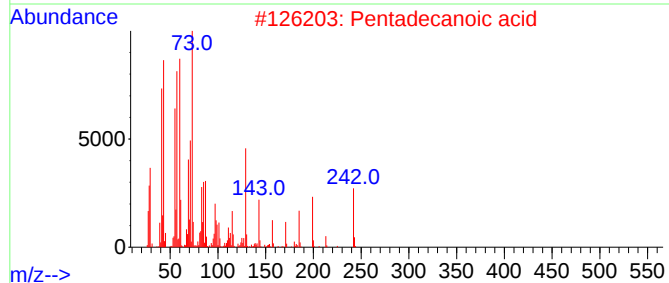
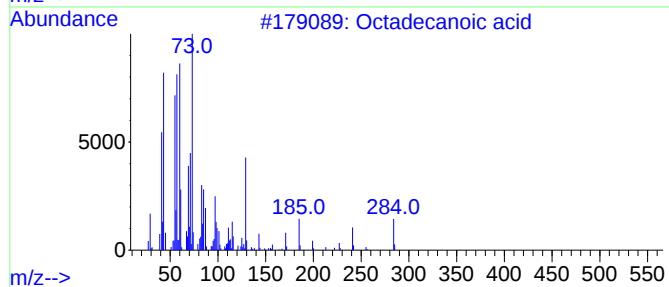
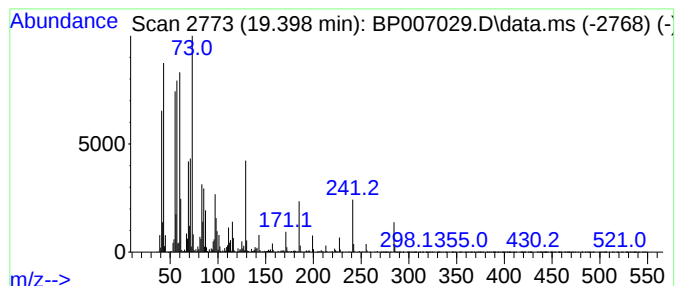
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	7.82 ng	1635280	Chrysene-d12	21.357

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	2.6	ng	233029	1	7.910	1772410	20.0
Ethanol, 1-(2-b...	10.493	2.7	ng	321474	2	10.704	2387860	20.0
2(3H)-Benzothia...	16.216	17.9	ng	3297660	4	17.281	3681880	20.0
n-Hexadecanoic ...	18.169	13.8	ng	2533530	4	17.281	3681880	20.0
Octadecanoic acid	19.398	7.8	ng	1635280	5	21.357	4179830	20.0