

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
 Data File : BP011818.D
 Acq On : 27 Sep 2022 16:35
 Operator : CG/JU
 Sample : N4841-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 252672-5

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-BP092122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011818.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	6	10	35	rVB	7584250	11987125	62.31%	10.832%
2	5.470	415	422	439	rBV	2295537	3536620	18.38%	3.196%
3	7.069	686	694	713	rBV	1250173	2121233	11.03%	1.917%
4	7.911	829	837	845	rBV	1189162	1927668	10.02%	1.742%
5	9.075	1027	1035	1054	rBV	3635624	6087519	31.64%	5.501%
6	10.499	1271	1277	1295	rBV	190867	439192	2.28%	0.397%
7	10.716	1307	1314	1332	rBV	1614958	2852217	14.83%	2.577%
8	13.181	1725	1733	1749	rBV	9286088	14297551	74.32%	12.920%
9	14.551	1957	1966	1978	rBV	2644164	3881588	20.18%	3.508%
10	16.045	2213	2220	2241	rBV	7873289	11298734	58.73%	10.210%
11	17.310	2428	2435	2441	rBV	3343674	4754657	24.71%	4.296%
12	18.192	2580	2585	2592	rBV	335124	647565	3.37%	0.585%
13	18.263	2592	2597	2610	rVB	8587772	10121165	52.61%	9.146%
14	19.422	2790	2794	2812	rBV	806508	1720876	8.94%	1.555%
15	19.863	2864	2869	2875	rBV	15170251	19238823	100.00%	17.385%
16	21.098	3076	3079	3090	rBV4	279369	491545	2.55%	0.444%
17	21.392	3124	3129	3139	rVB	4109507	5322766	27.67%	4.810%
18	21.516	3145	3150	3164	rBV	2824028	4421424	22.98%	3.995%
19	23.833	3538	3544	3554	rVB2	2694558	5516235	28.67%	4.985%

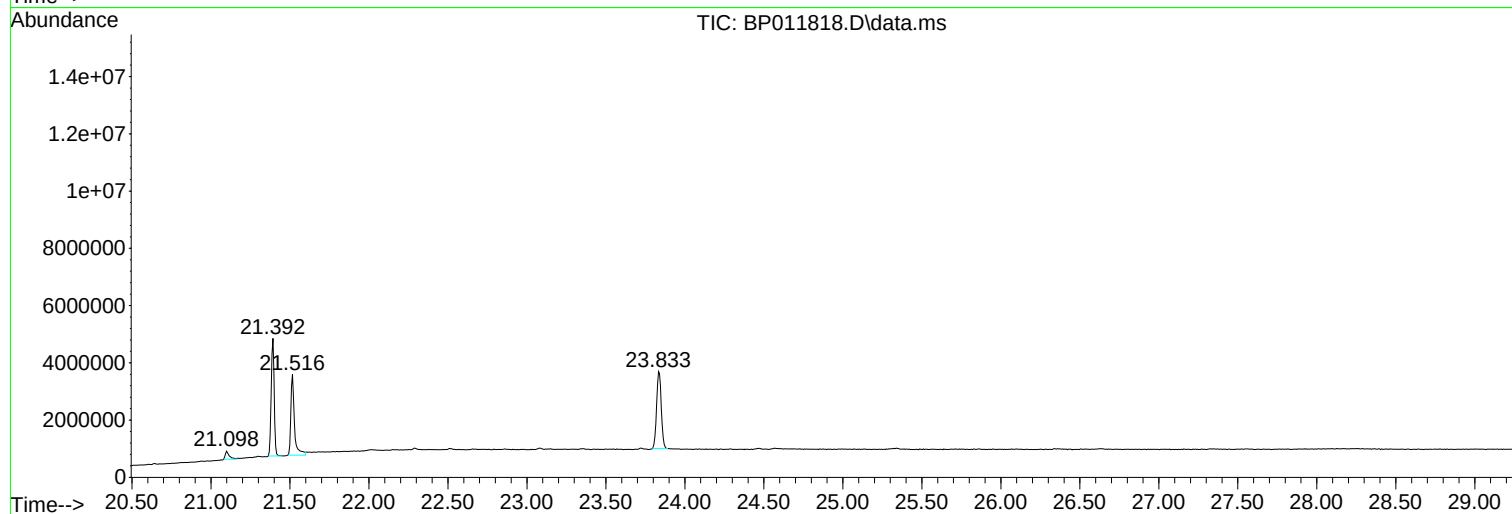
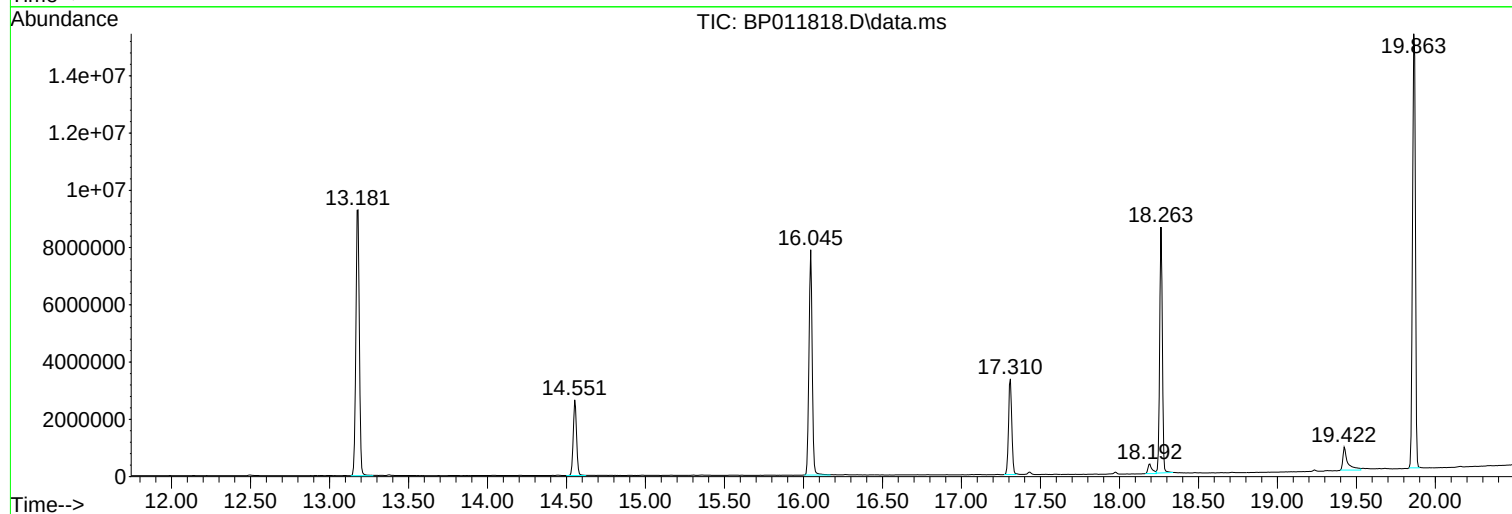
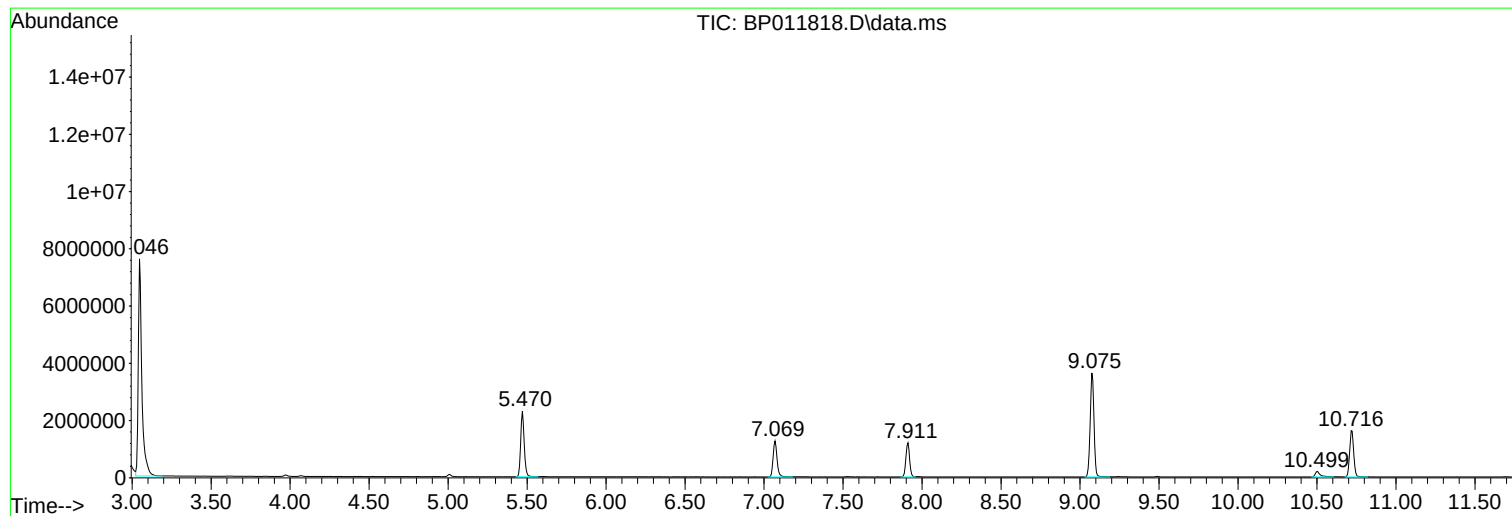
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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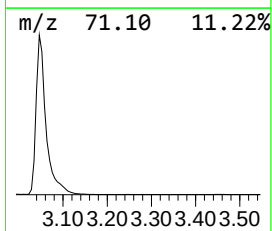
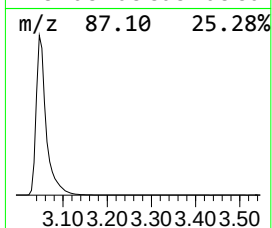
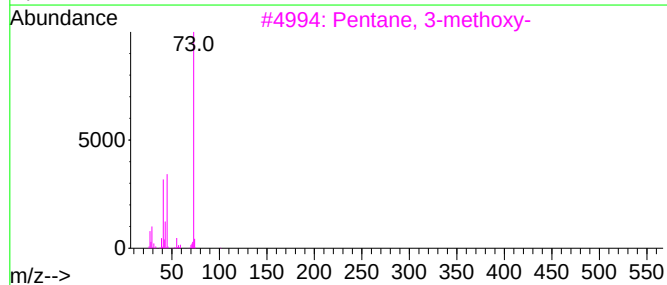
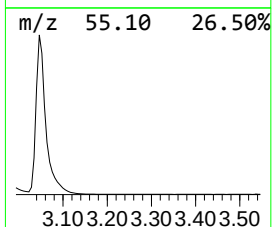
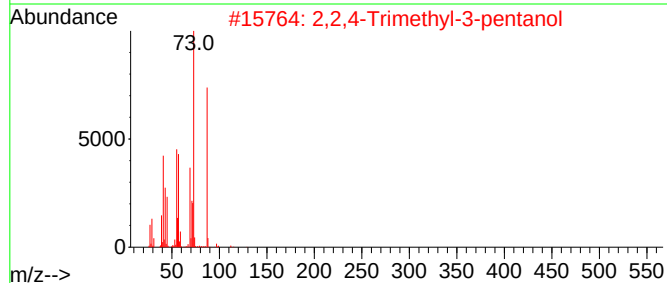
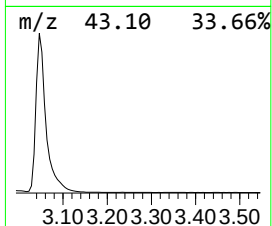
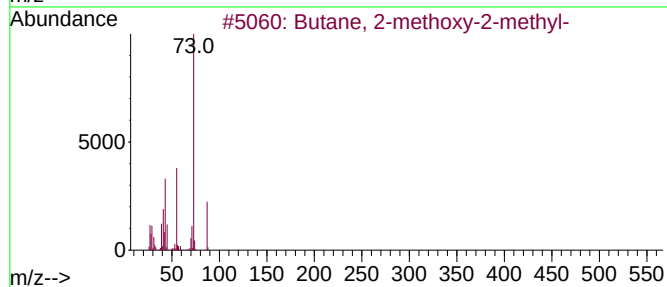
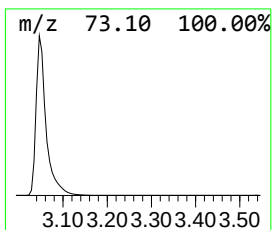
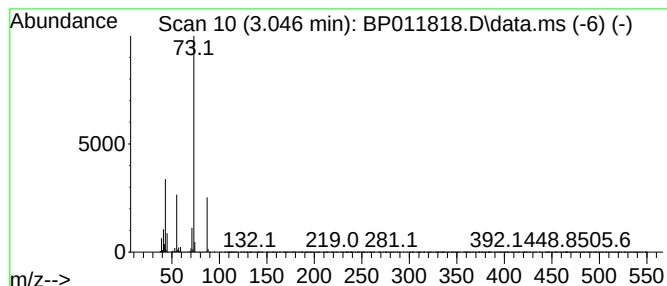
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	124.37 ng	11987100	1,4-Dichlorobenzene-d4	7.911

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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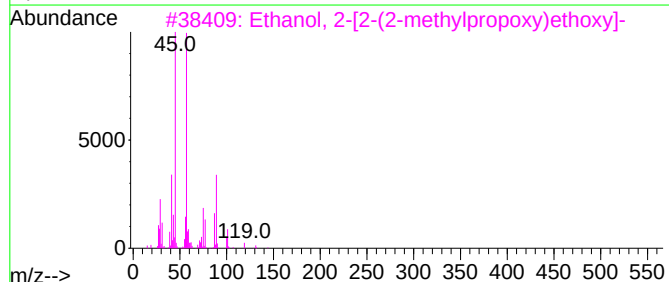
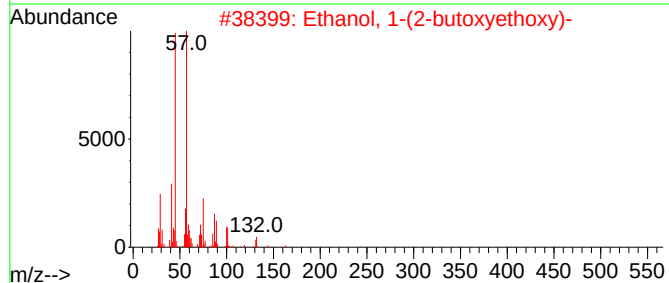
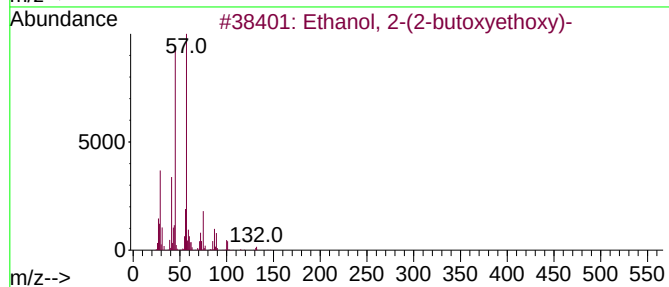
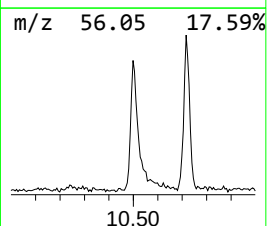
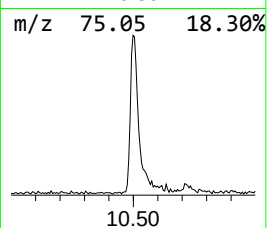
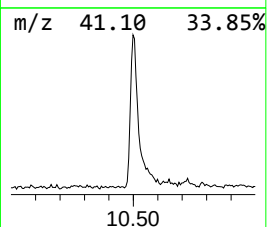
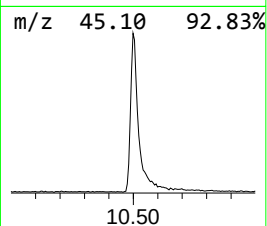
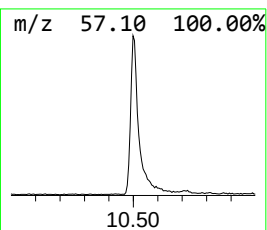
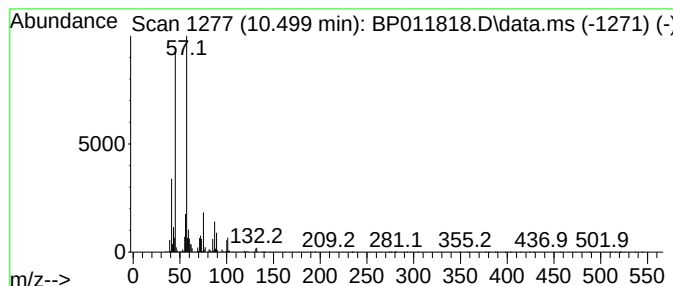
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.499	3.08 ng	439192	Naphthalene-d8	10.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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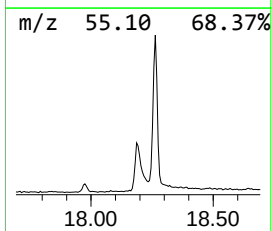
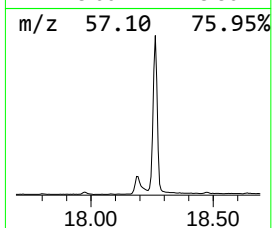
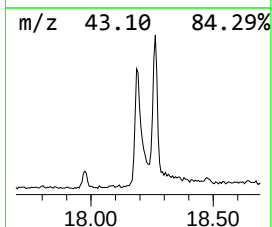
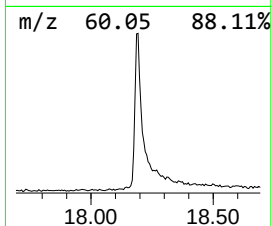
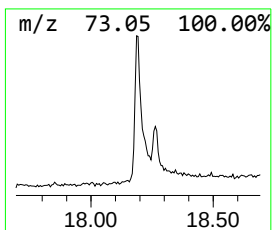
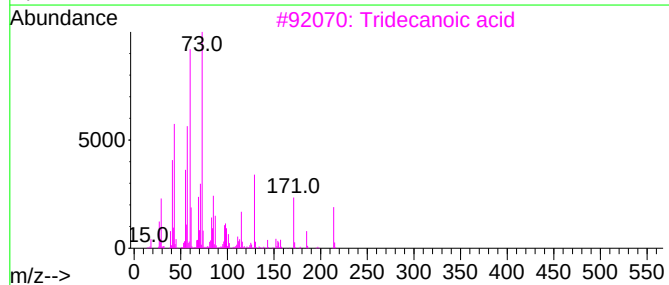
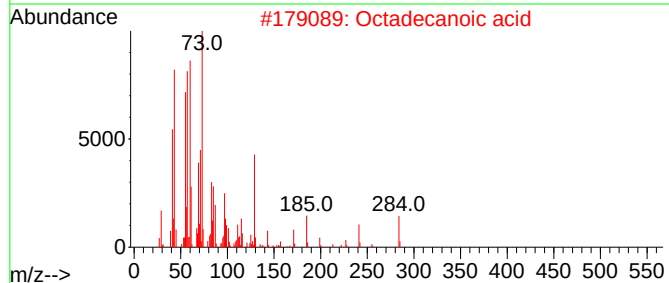
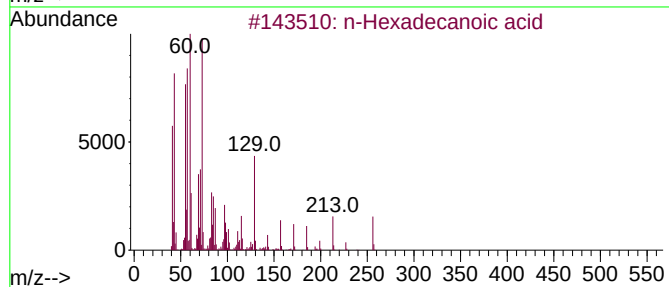
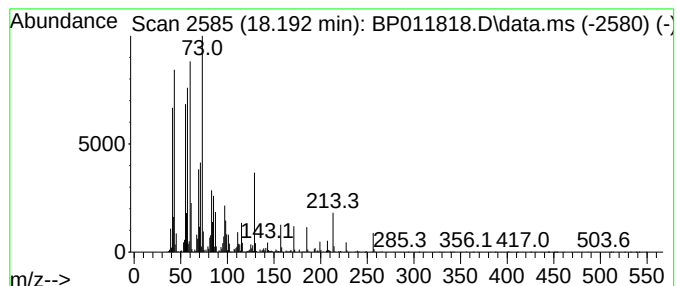
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.192	2.72 ng	647565	Phenanthrene-d10		17.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Octadecanoic acid		284	C18H36O2	000057-11-4	87
3	Tridecanoic acid		214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	Pentadecanoic acid		242	C15H30O2	001002-84-2	68



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Instrument :
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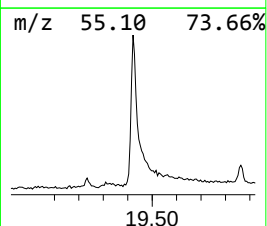
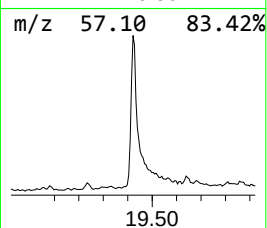
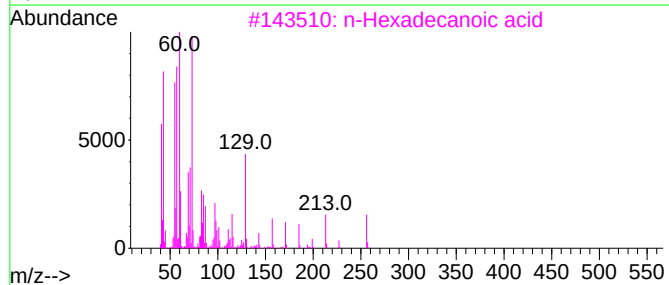
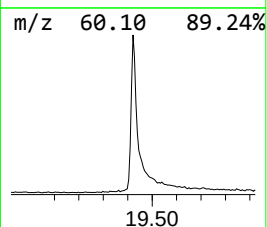
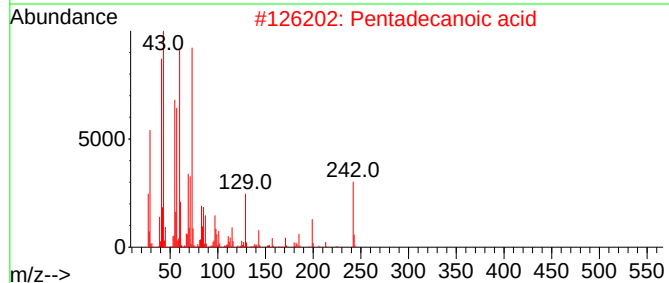
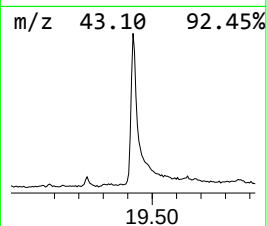
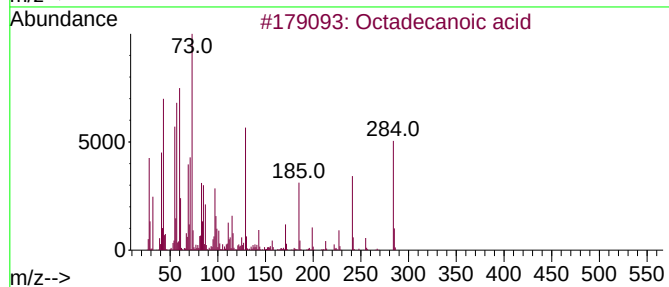
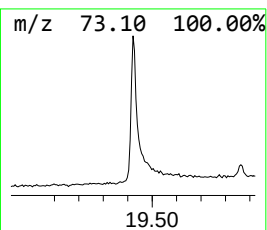
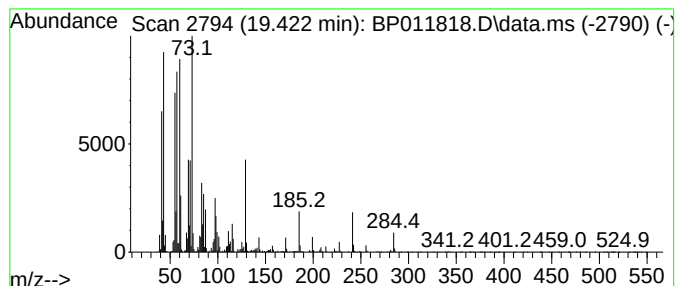
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	6.47 ng	1720880	Chrysene-d12	21.392

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	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87



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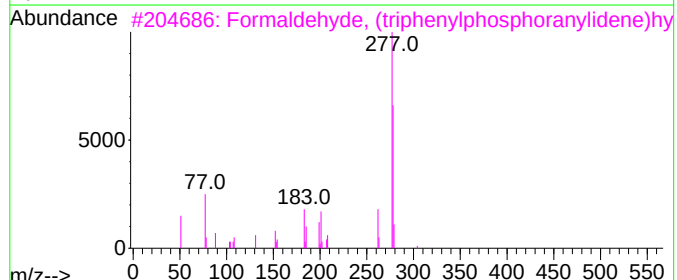
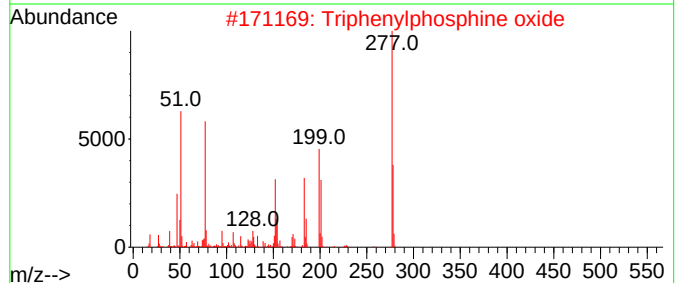
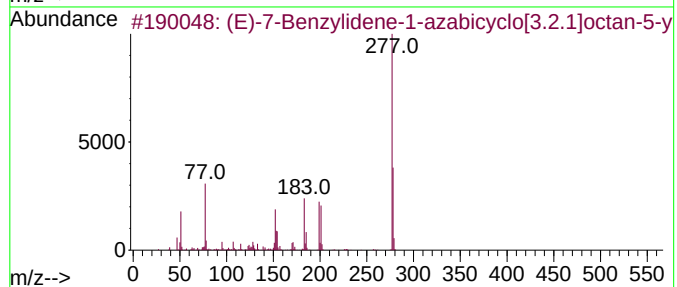
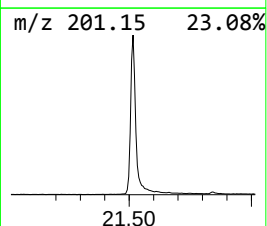
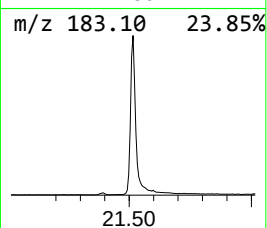
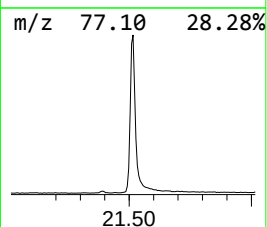
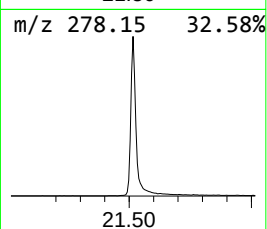
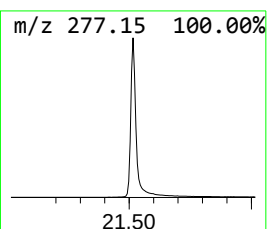
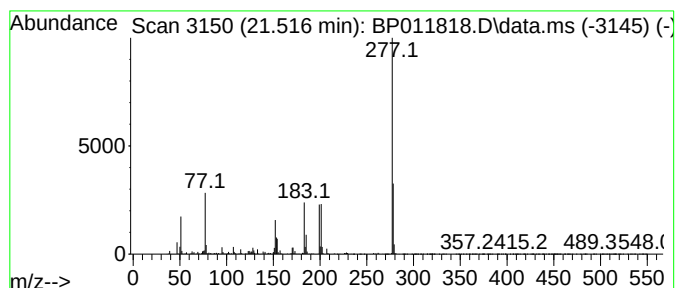
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Peak Number 5 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.516	16.61 ng	4421420	Chrysene-d12		21.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...		293	C15H19NO3S	1000483-83-4	95
2	Triphenylphosphine oxide		278	C18H15OP	000791-28-6	91
3	Formaldehyde, (triphenylphosphor...		304	C19H17N2P	015990-54-2	45
4	4-Nitro-4'-methyldiphenylsulfone		277	C13H11NO4S	004094-37-5	38
5	Carbazol-1-one, 1,2,3,4-tetrahyd...		277	C18H15NO2	299962-12-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.046	124.4	ng	11987100	1	7.911	1927670	20.0
Ethanol, 2-(2-b...	10.499	3.1	ng	439192	2	10.716	2852220	20.0
n-Hexadecanoic ...	18.192	2.7	ng	647565	4	17.310	4754660	20.0
Octadecanoic acid	19.422	6.5	ng	1720880	5	21.392	5322770	20.0
(E)-7-Benzylide...	21.516	16.6	ng	4421420	5	21.392	5322770	20.0