

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
 Data File : BP008733.D
 Acq On : 07 Jan 2022 19:02
 Operator : CG/JU
 Sample : N1065-14
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 AMI-4

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-BP010622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008733.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.064	9	13	33	rVB	1633234	2455790	13.30%	2.615%
2	5.452	412	419	431	rBV	3912237	6173232	33.43%	6.574%
3	7.040	681	689	708	rBV	3757077	6314088	34.19%	6.724%
4	7.869	822	830	838	rBV	1214994	1954520	10.59%	2.082%
5	9.028	1018	1027	1039	rBV	2373595	4088422	22.14%	4.354%
6	10.452	1261	1269	1288	rBV	357438	752199	4.07%	0.801%
7	10.669	1299	1306	1317	rBV	1571998	2771651	15.01%	2.952%
8	13.134	1718	1725	1742	rBV	6751338	10464939	56.67%	11.145%
9	14.345	1923	1931	1941	rBV	75946	247547	1.34%	0.264%
10	14.504	1952	1958	1980	rVB	2454896	3864309	20.93%	4.115%
11	15.998	2205	2212	2239	rBV	5307429	8365484	45.30%	8.909%
12	17.257	2420	2426	2440	rBV	3152476	4935903	26.73%	5.257%
13	18.157	2574	2579	2587	rBV	429084	702326	3.80%	0.748%
14	19.386	2785	2788	2798	rBV	256476	423837	2.30%	0.451%
15	19.622	2825	2828	2836	rVB	113295	185599	1.01%	0.198%
16	19.822	2856	2862	2870	rBV	14746904	18464957	100.00%	19.665%
17	21.063	3069	3073	3080	rBV	1203416	1524436	8.26%	1.623%
18	21.227	3097	3101	3104	rBV3	520071	970013	5.25%	1.033%
19	21.351	3116	3122	3126	rBV	4896424	6364322	34.47%	6.778%
20	21.469	3137	3142	3147	rBV	4211001	6028232	32.65%	6.420%
21	23.774	3527	3534	3545	rVB	3270396	6847563	37.08%	7.292%

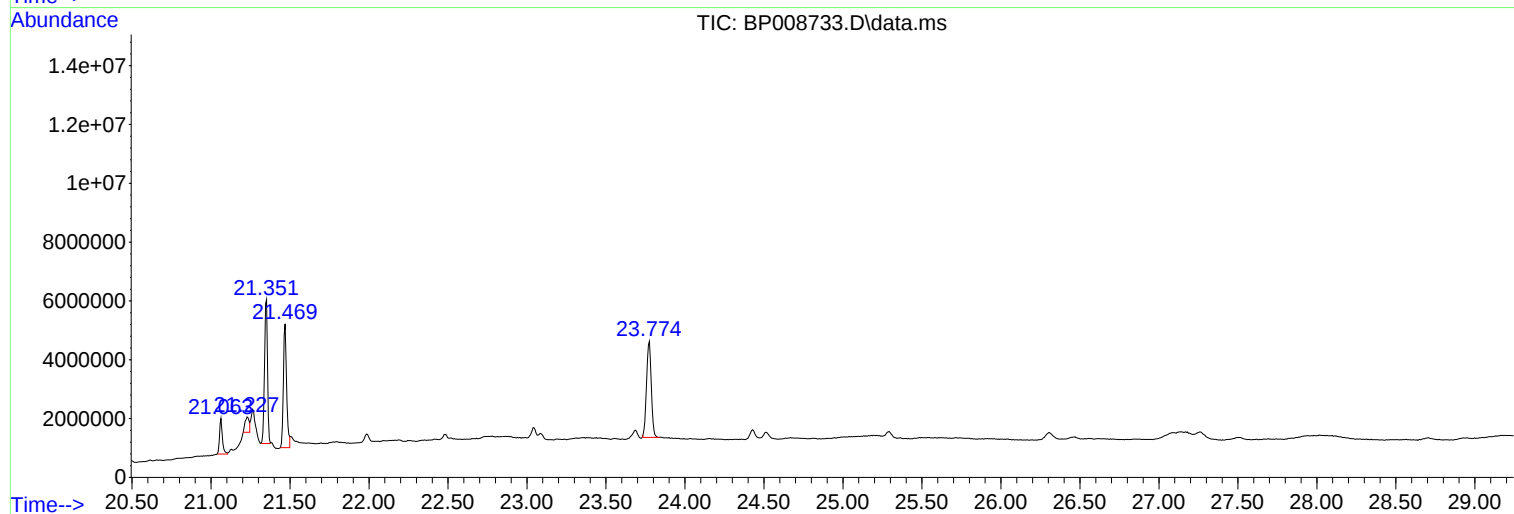
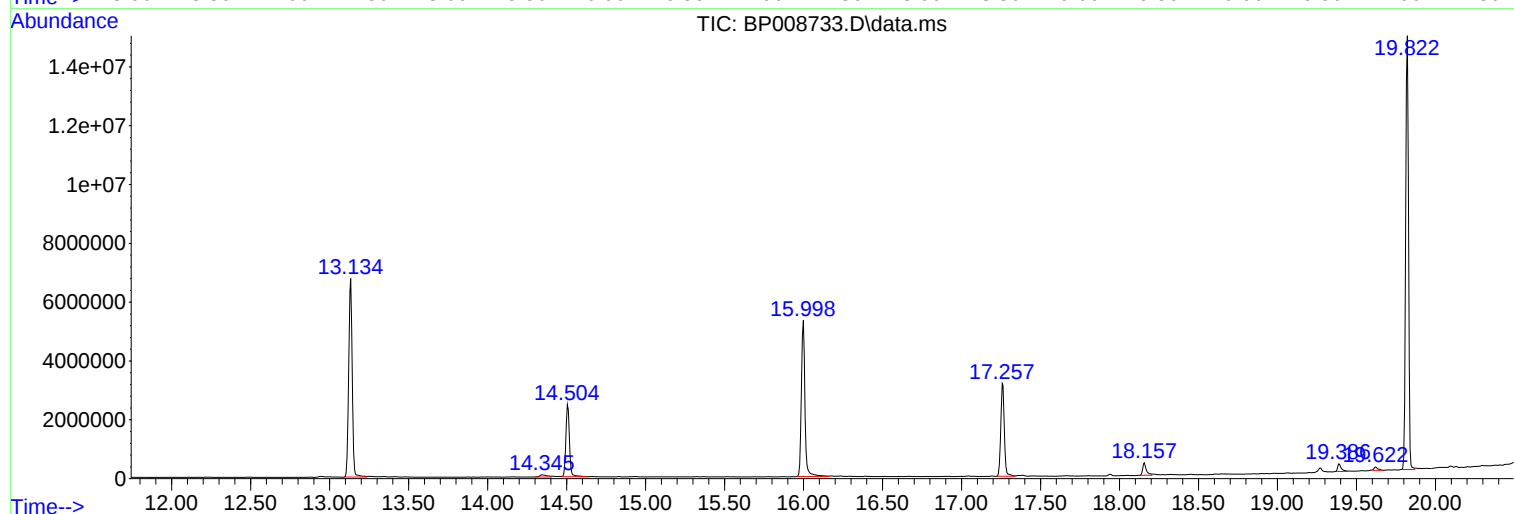
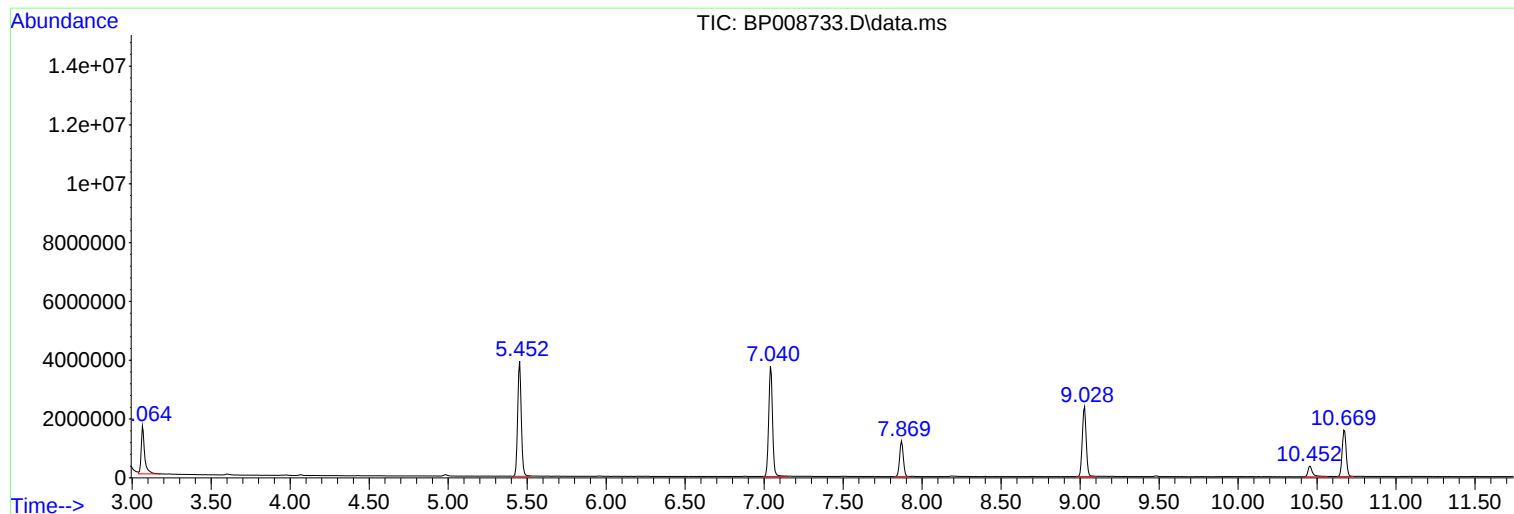
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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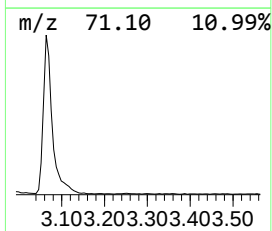
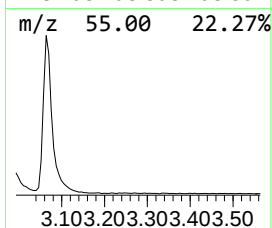
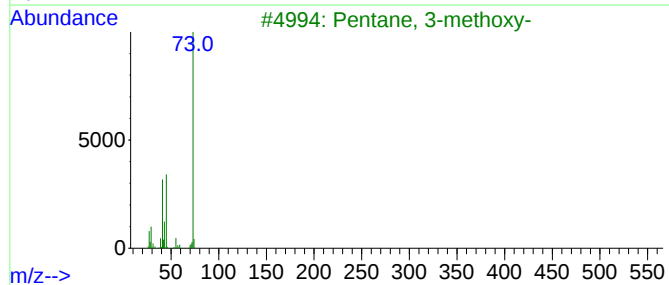
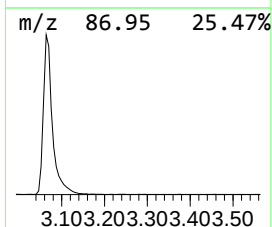
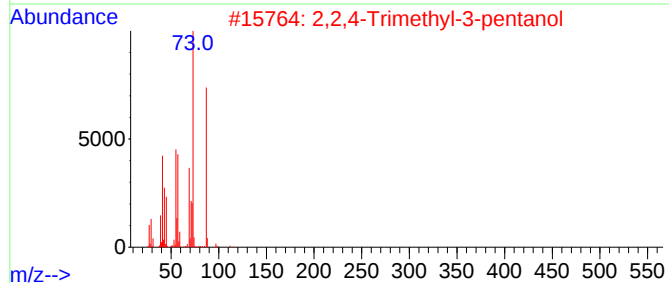
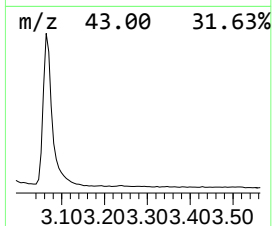
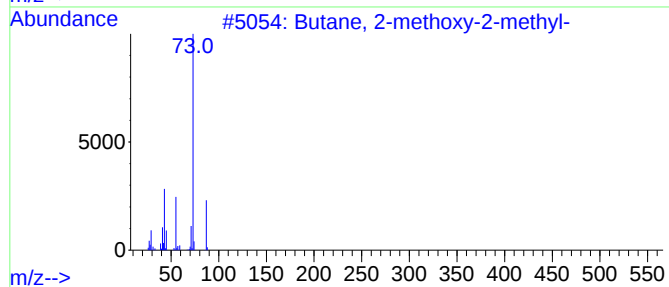
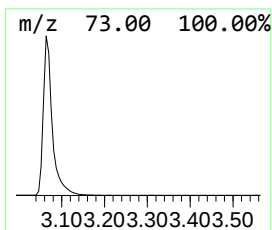
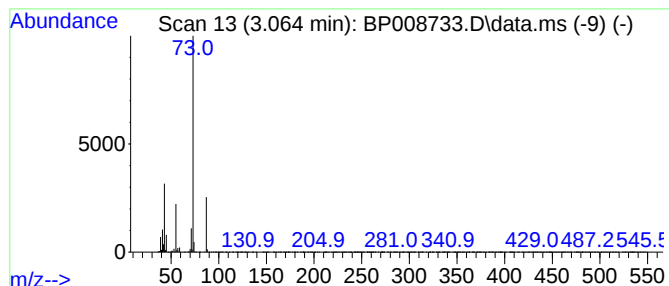
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.064	25.13 ng	2455790	1,4-Dichlorobenzene-d4	7.869

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	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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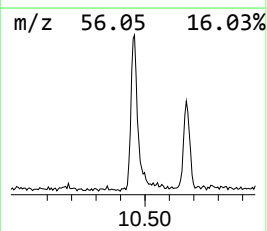
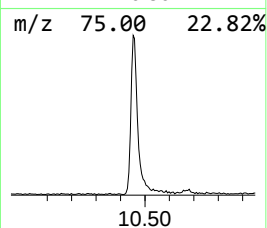
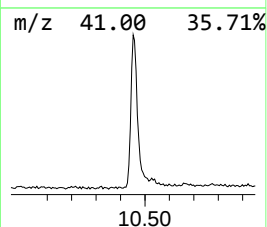
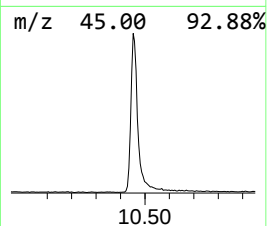
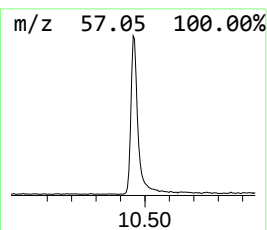
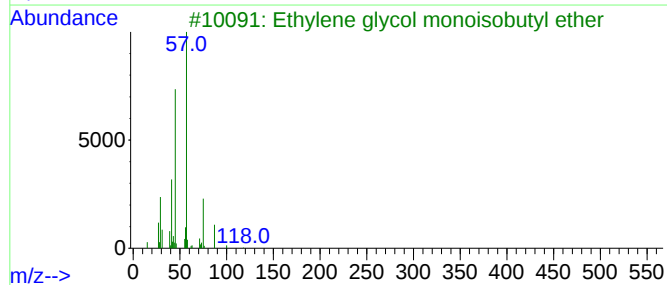
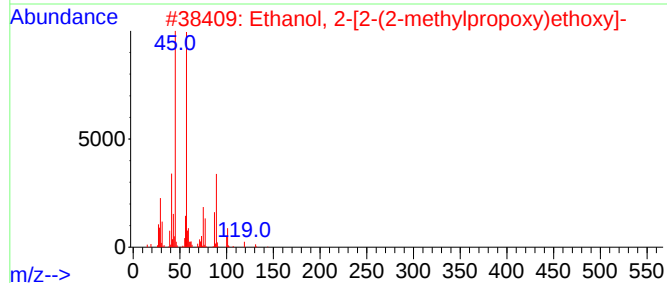
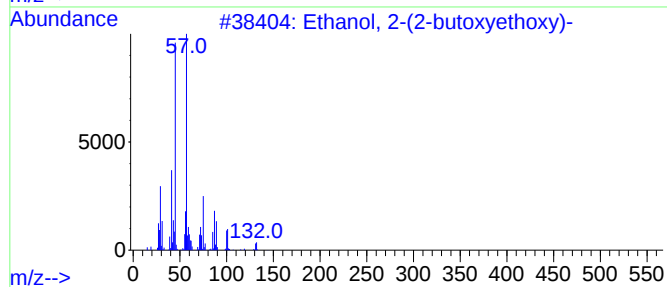
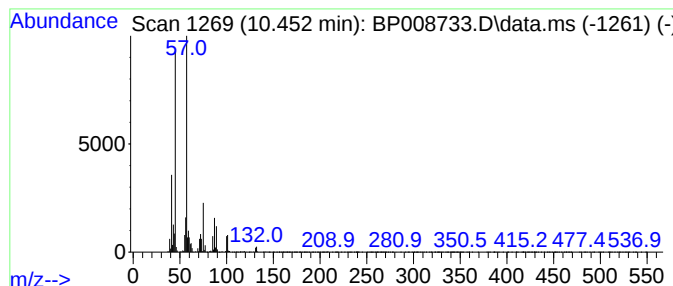
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	5.43 ng	752199	Naphthalene-d8	10.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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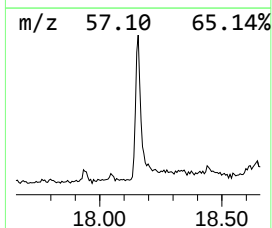
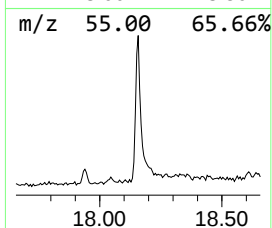
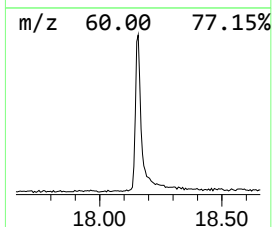
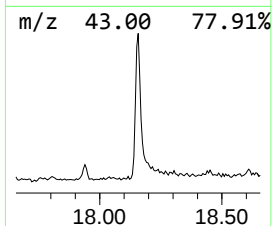
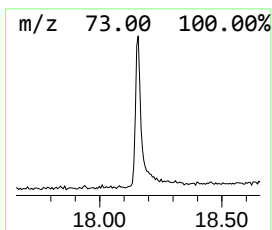
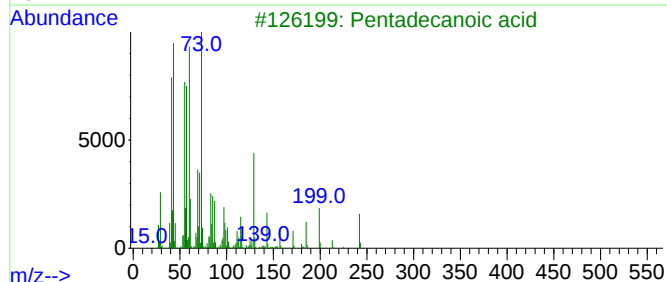
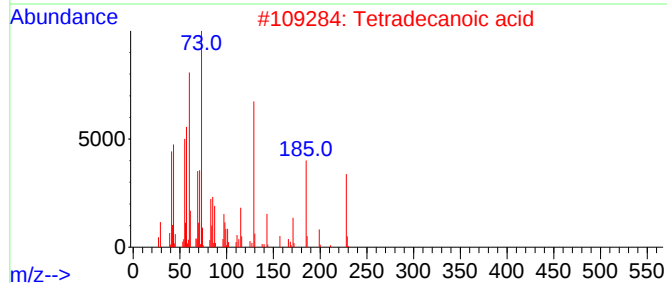
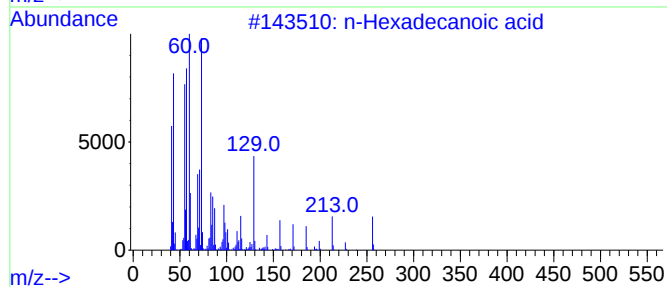
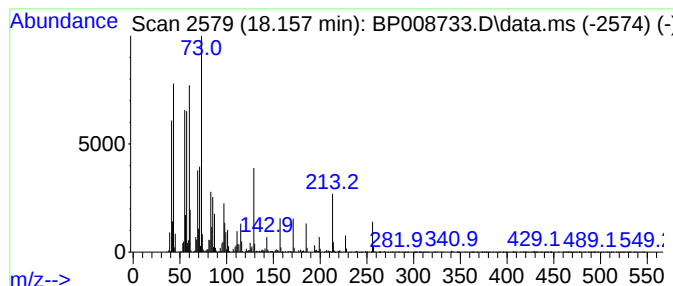
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	2.85 ng	702326	Phenanthrene-d10	17.257

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	91
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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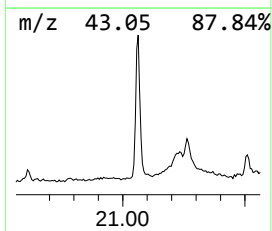
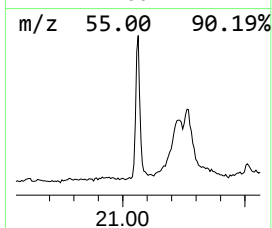
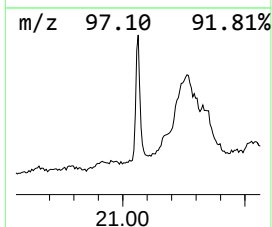
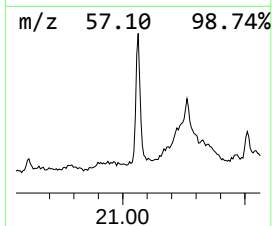
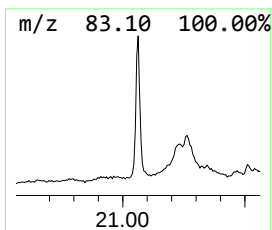
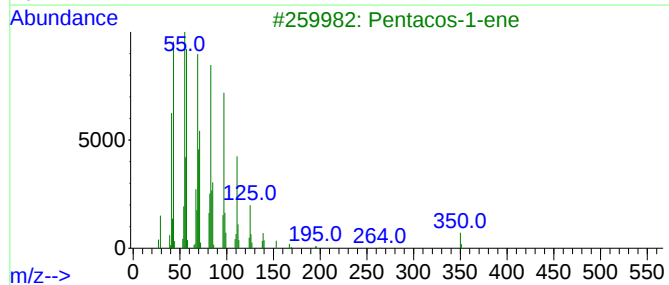
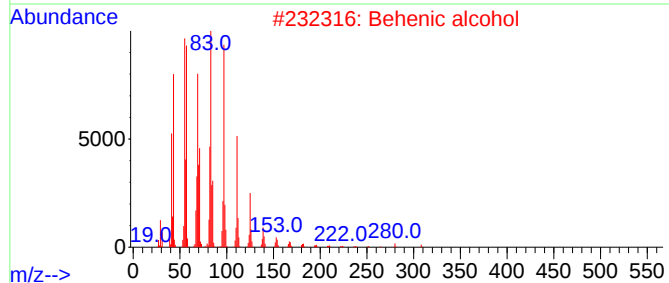
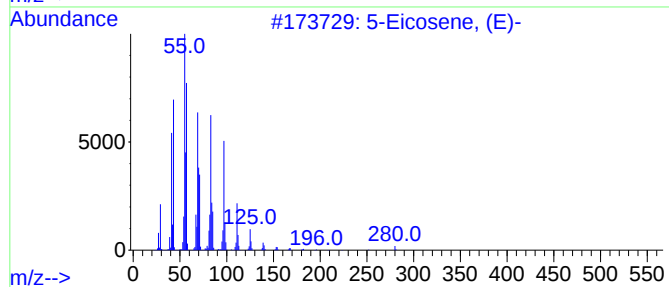
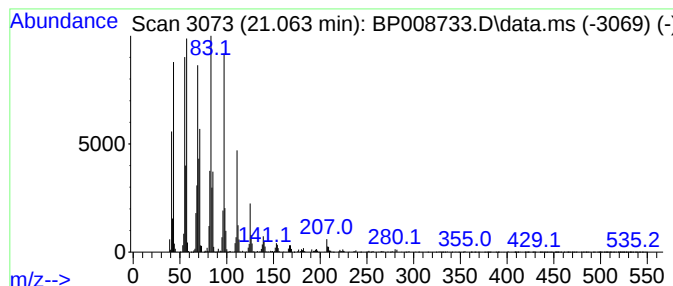
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	4.79 ng	1524440	Chrysene-d12	21.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	Behenic alcohol		326	C22H46O	000661-19-8	95
3	Pentacos-1-ene		350	C25H50	016980-85-1	94
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	Nonacos-1-ene		406	C29H58	018835-35-3	94



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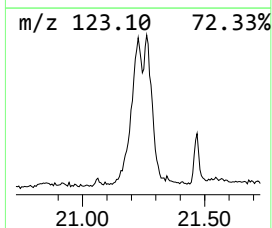
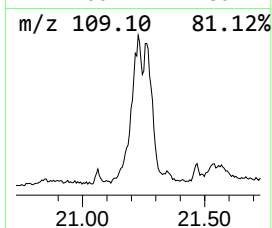
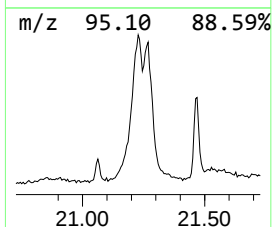
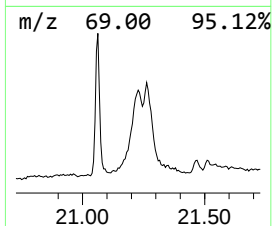
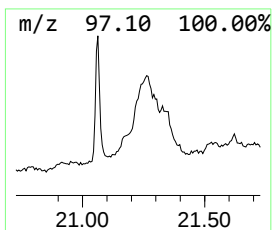
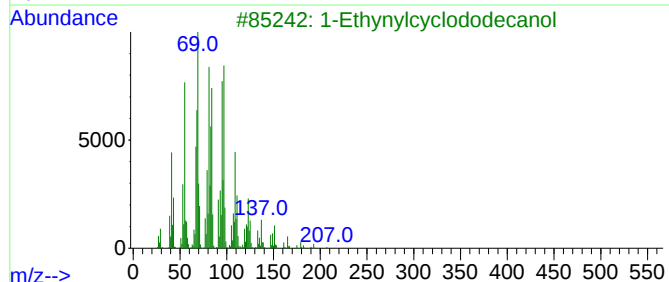
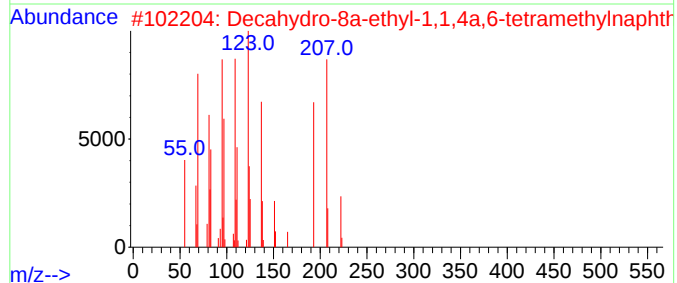
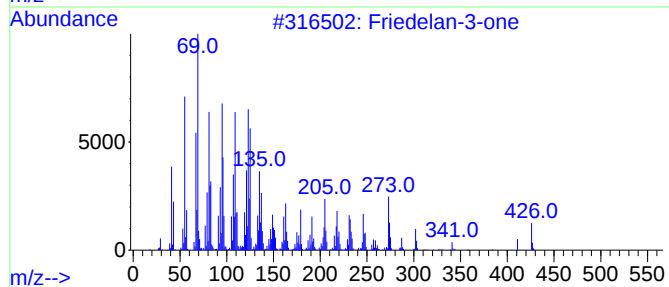
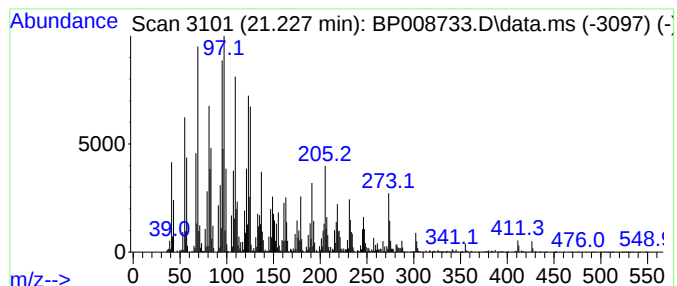
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Friedelan-3-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	3.05 ng	970013	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	89
2			Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	60
3			1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	46
4			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	41
5			1-Formyl-2,2-dimethyl-3-cis-(2-m...	220	C15H24O	1000144-10-0	38



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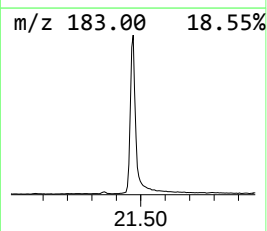
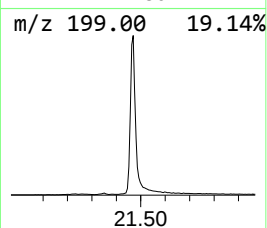
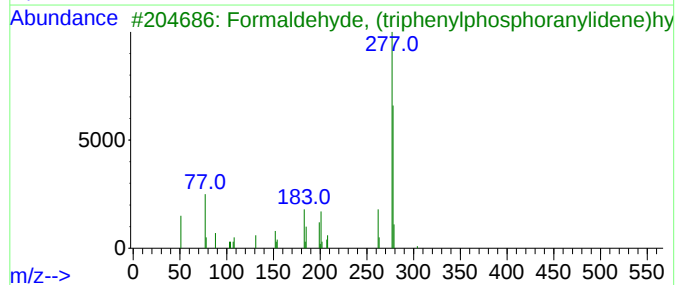
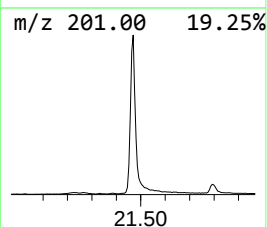
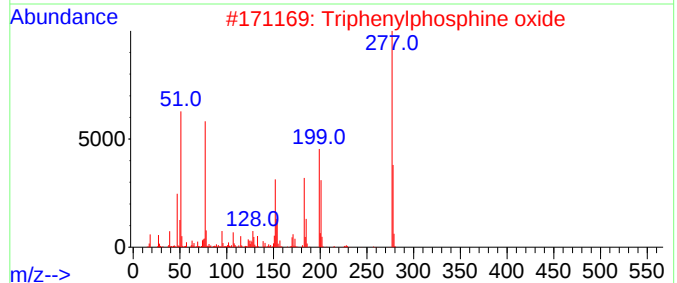
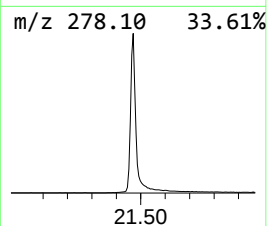
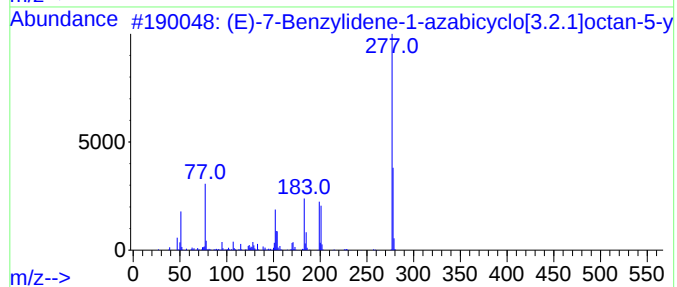
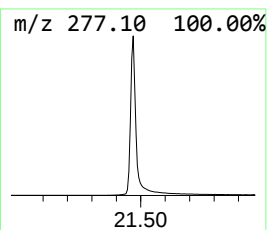
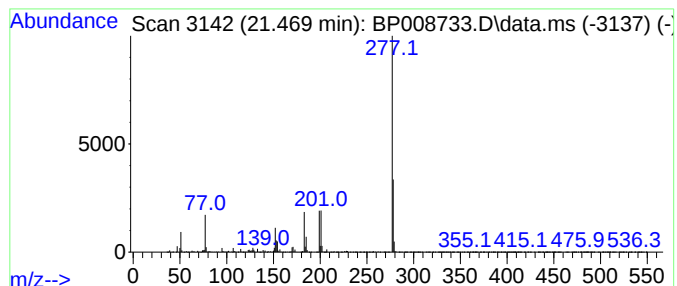
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.469	18.94 ng	6028230	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl	293	C15H19NO3S	1000483-83-4	91		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	74		
3	Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	37		
4	3-(3,4-Dichlorophenyl)-2-thioxo-1,2,3,4-tetrahydropyridine	277	C9H5Cl2NOS2	017046-34-3	32		
5	2-Phenyl-6-(trifluoromethyl)-1H-benzimidazole	277	C15H10F3NO	1000387-59-3	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008733.D
Acq On : 07 Jan 2022 19:02
Operator : CG/JU
Sample : N1065-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
AMI-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	3.064	25.1	ng	2455790	1	7.869	1954520	20.0
Ethanol, 2-(2-b...	10.451	5.4	ng	752199	2	10.669	2771650	20.0
n-Hexadecanoic ...	18.157	2.9	ng	702326	4	17.257	4935900	20.0
5-Eicosene, (E)-	21.063	4.8	ng	1524440	5	21.351	6364320	20.0
Friedelan-3-one	21.227	3.0	ng	970013	5	21.351	6364320	20.0
(E)-7-Benzylide...	21.469	18.9	ng	6028230	5	21.351	6364320	20.0