

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
 Data File : BP007037.D
 Acq On : 17 Sep 2021 21:19
 Operator : CG/JU
 Sample : M3791-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-CB-03-(1.0)

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: BP007037.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	324	329	339	rBV	167464	250405	1.31%	0.305%
2	5.222	357	363	370	rVB	132098	196890	1.03%	0.240%
3	5.475	400	406	420	rBV	2500527	3704866	19.34%	4.510%
4	7.069	669	677	693	rBV	1429992	2269557	11.85%	2.763%
5	7.905	811	819	829	rBV	1118494	1796835	9.38%	2.187%
6	9.069	1005	1017	1028	rBV	3240908	5461952	28.51%	6.649%
7	10.487	1250	1258	1274	rBV	1203249	2048975	10.69%	2.494%
8	10.704	1288	1295	1303	rBV	1479633	2396008	12.51%	2.917%
9	13.163	1705	1713	1728	rBV	8657307	13102837	68.39%	15.949%
10	13.440	1753	1760	1768	rBV	294403	447746	2.34%	0.545%
11	14.534	1938	1946	1953	rBV	2105735	3120529	16.29%	3.798%
12	15.486	2103	2108	2126	rVB	209943	353968	1.85%	0.431%
13	15.969	2185	2190	2193	rBV	147914	213019	1.11%	0.259%
14	16.022	2193	2199	2211	rVB	6420474	9525511	49.72%	11.595%
15	16.210	2224	2231	2244	rBV	1624550	2614359	13.65%	3.182%
16	17.280	2406	2413	2419	rBV	2581767	3633728	18.97%	4.423%
17	18.169	2558	2564	2573	rBV	700208	1062139	5.54%	1.293%
18	19.080	2716	2719	2723	rVB	504869	536167	2.80%	0.653%
19	19.398	2769	2773	2786	rBV	231692	356343	1.86%	0.434%
20	19.833	2842	2847	2858	rBV	15042035	19158990	100.00%	23.321%
21	20.104	2889	2893	2897	rBV	196379	258673	1.35%	0.315%
22	20.457	2950	2953	2959	rVB	278741	338792	1.77%	0.412%
23	21.069	3054	3057	3063	rBV2	264656	345436	1.80%	0.420%
24	21.274	3088	3092	3097	rBV	271572	321345	1.68%	0.391%
25	21.357	3101	3106	3116	rBV	3265681	4200996	21.93%	5.114%
26	23.768	3509	3516	3528	rVB2	2210464	4436350	23.16%	5.400%

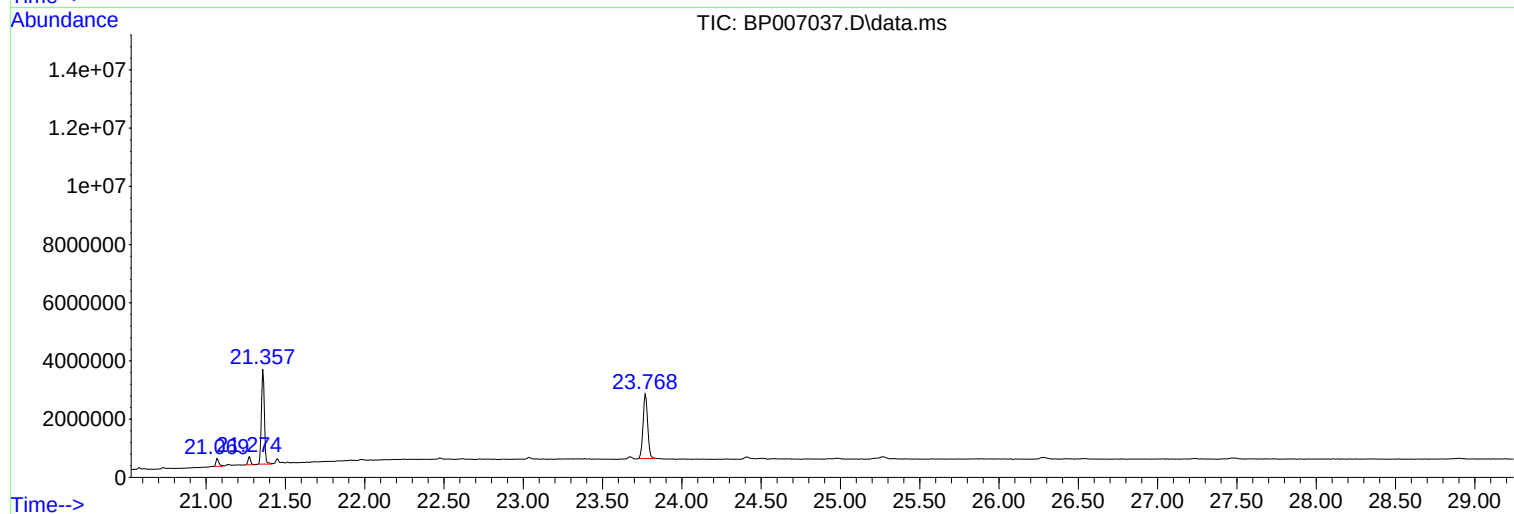
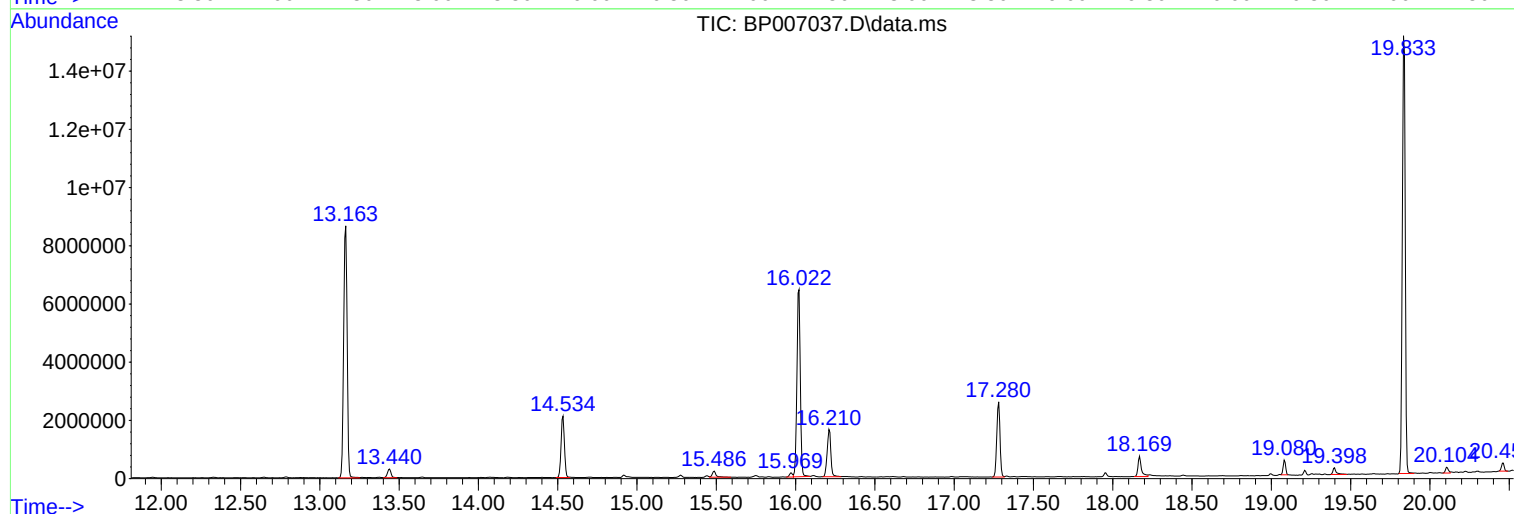
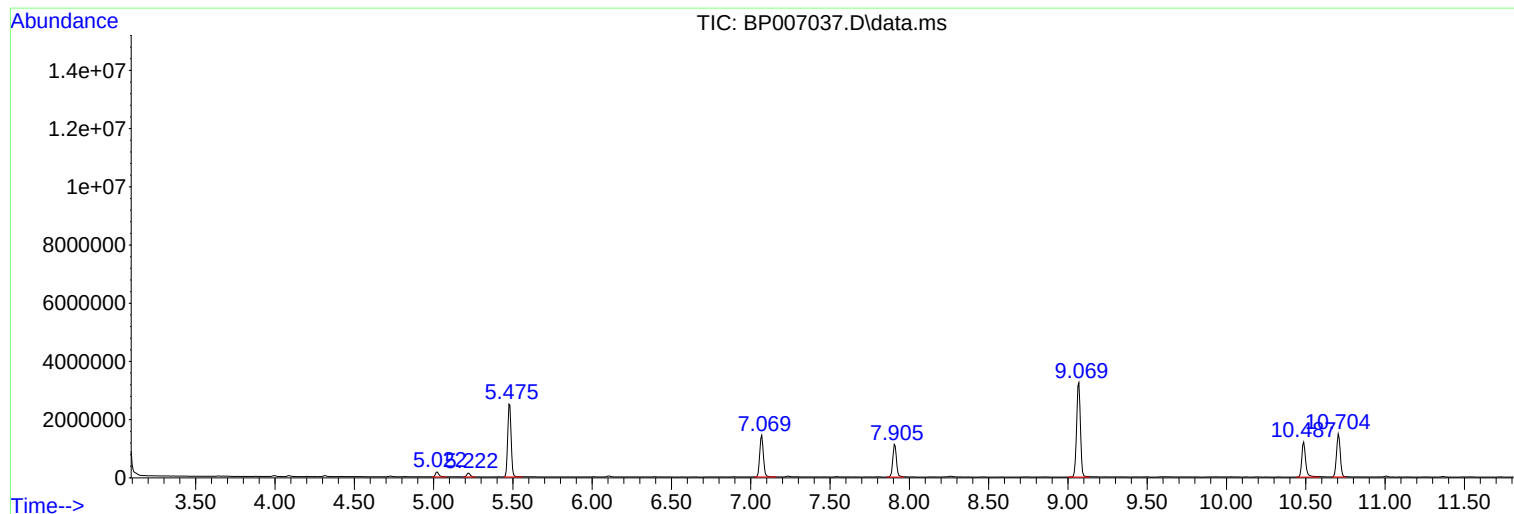
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ClientSampleId :
SW-CB-03-(1.0)

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



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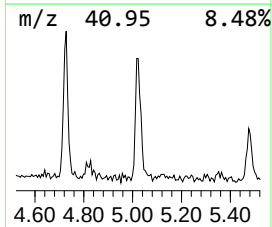
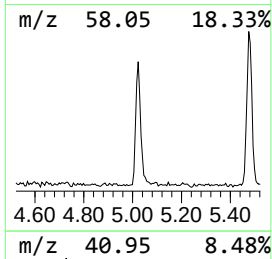
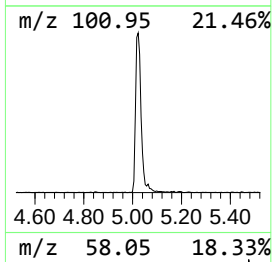
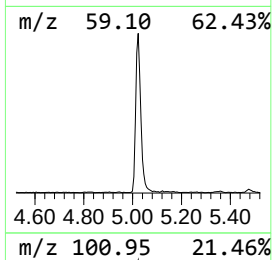
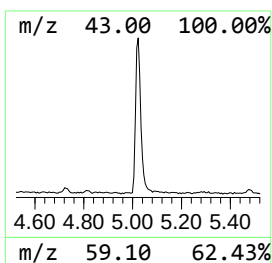
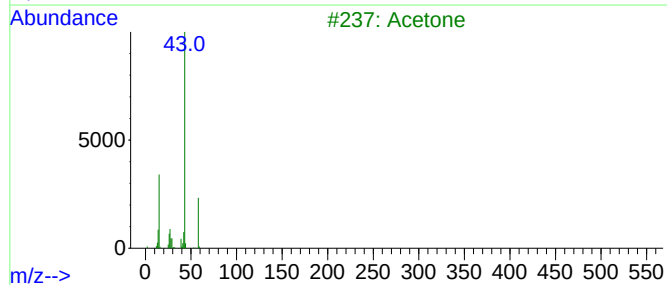
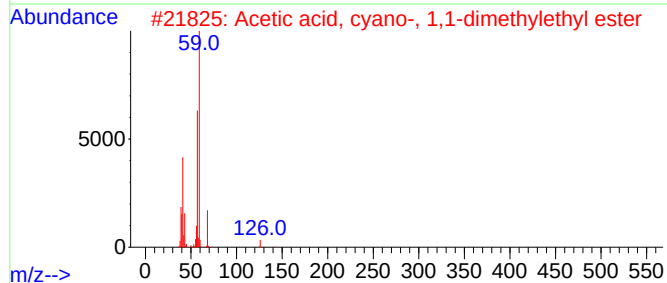
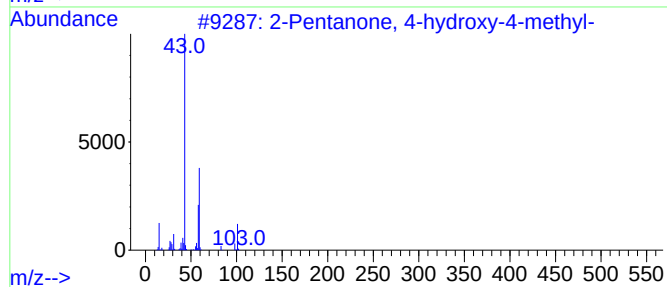
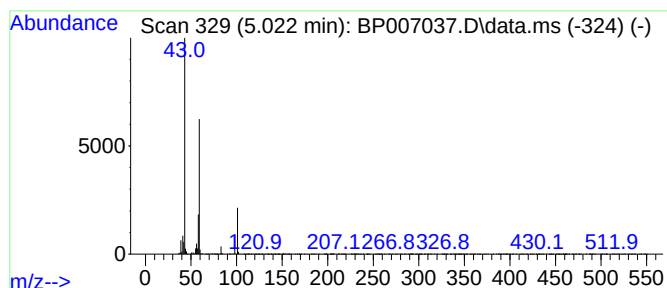
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	2.79 ng	250405	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	Acetone	58	C3H6O	000067-64-1	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Guanidine	59	CH5N3	000113-00-8	9		



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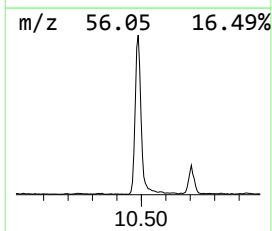
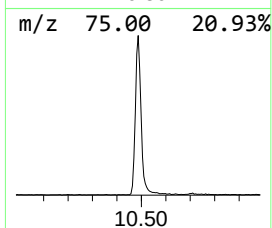
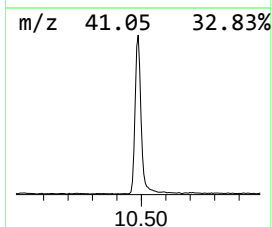
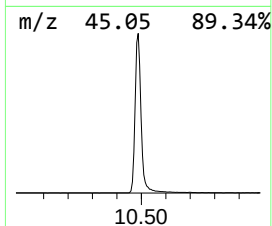
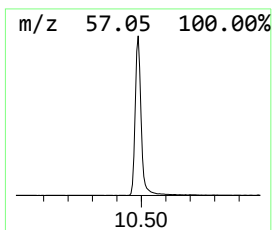
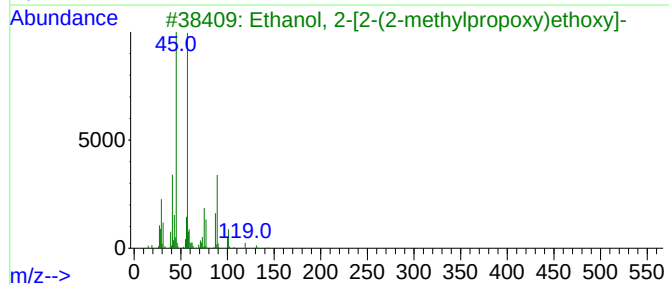
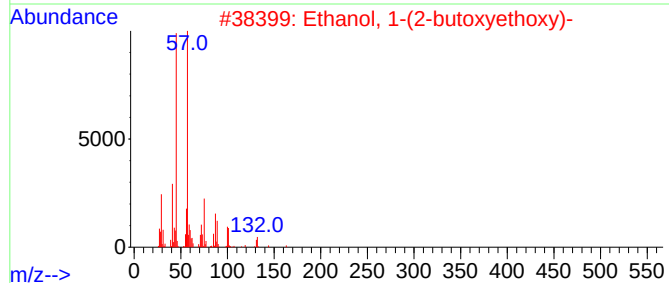
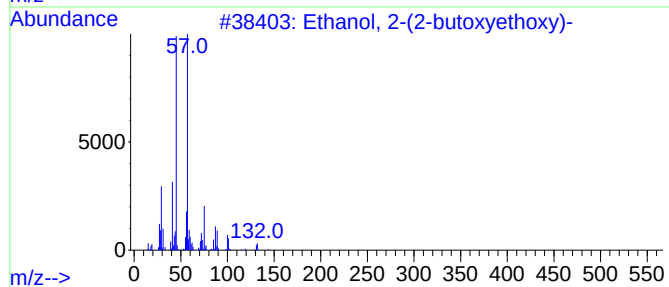
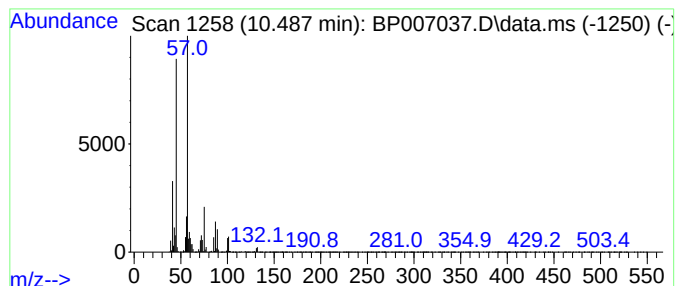
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	17.10 ng	2048980	Naphthalene-d8	10.704

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	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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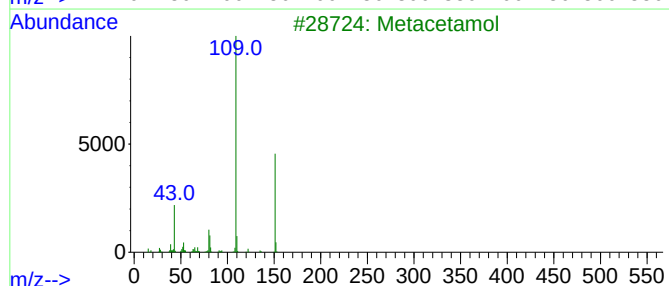
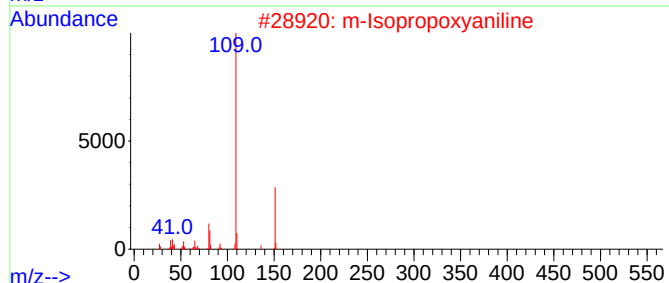
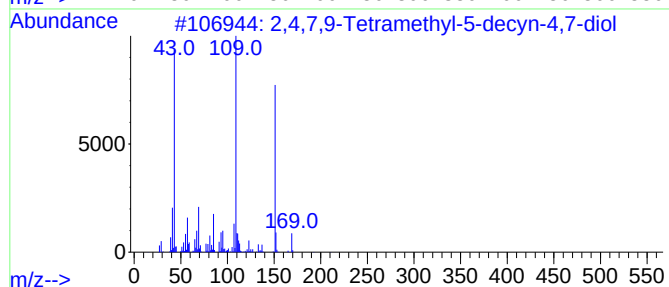
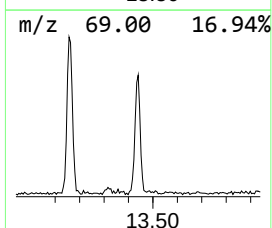
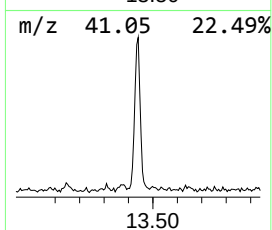
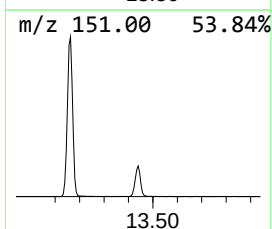
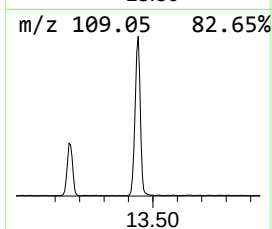
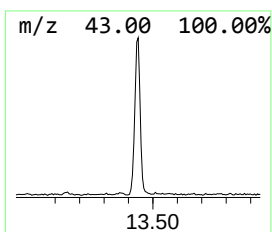
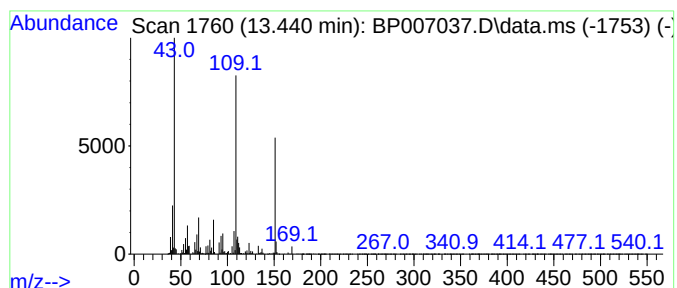
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.440	2.87 ng	447746	Acenaphthene-d10	14.534	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
3	Metacetamol	151	C8H9NO2	000621-42-1	53
4	Acetaminophen	151	C8H9NO2	000103-90-2	53
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53



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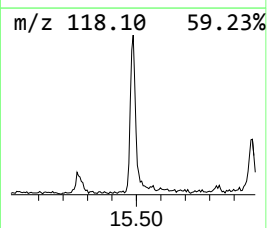
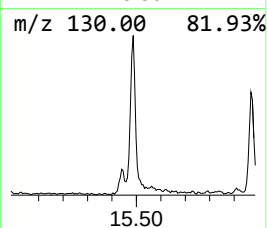
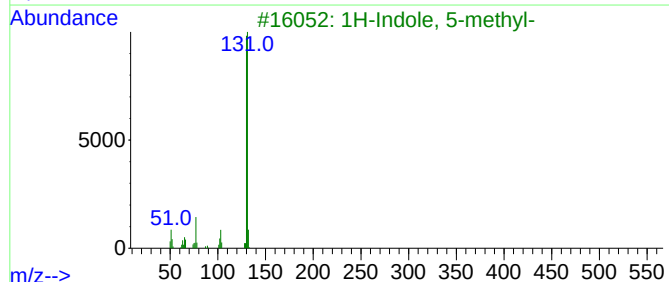
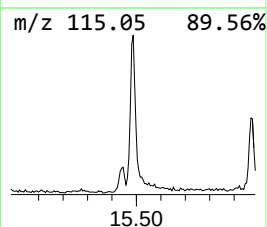
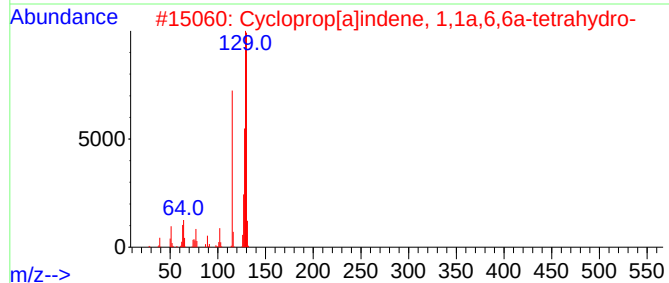
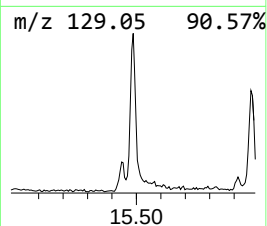
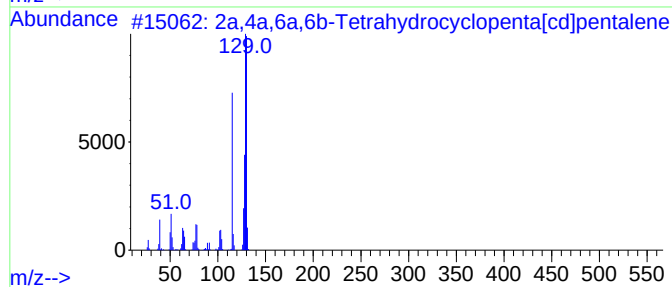
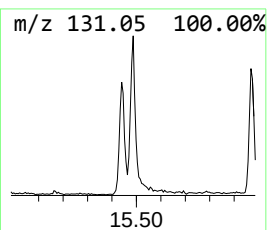
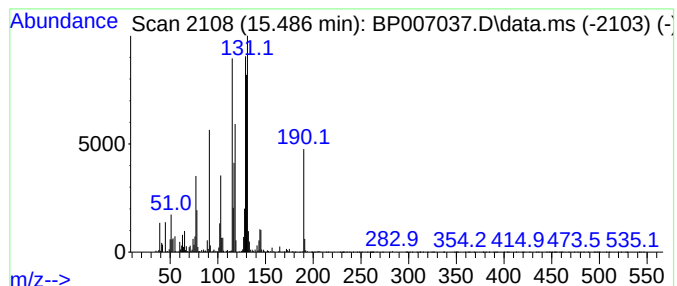
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Peak Number 5 unknown15.486 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	2.27 ng	353968	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	43		
2	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	43		
3	1H-Indole, 5-methyl-	131	C9H9N	000614-96-0	38		
4	Isoquinoline, 3,4-dihydro-	131	C9H9N	003230-65-7	38		
5	1H-Indole, 7-methyl-	131	C9H9N	000933-67-5	38		



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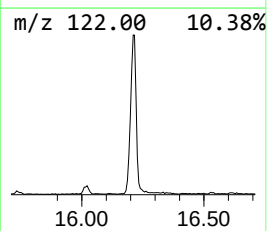
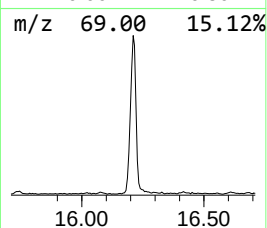
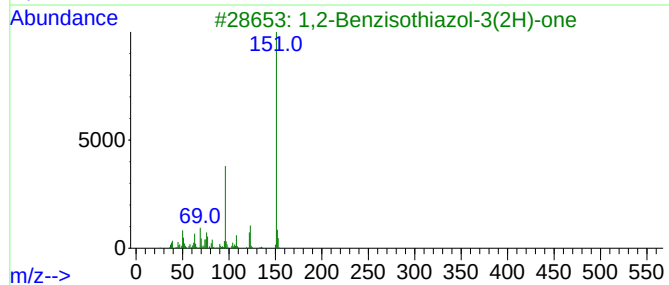
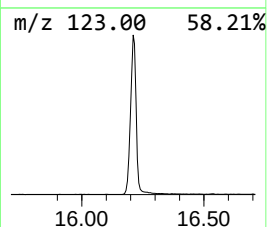
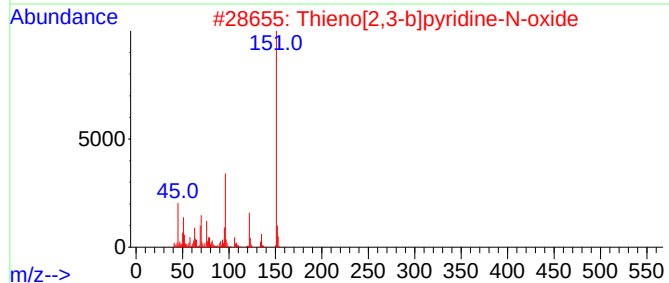
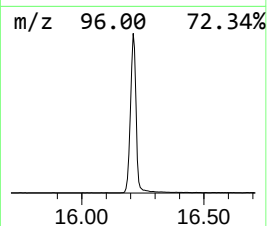
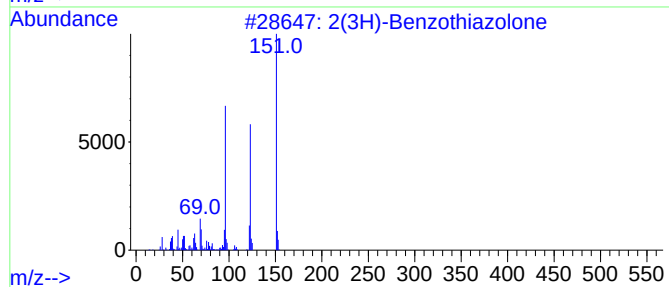
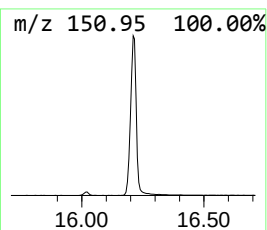
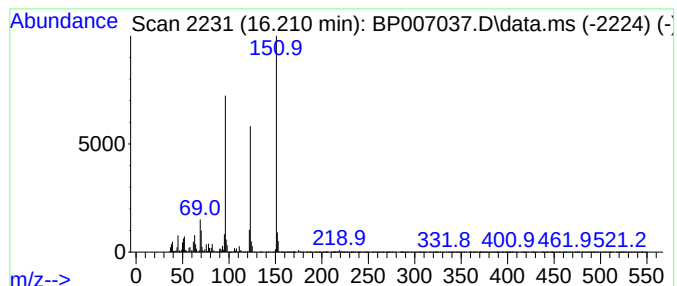
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.210	14.39 ng	2614360	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2			Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	53
3			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	50
4			6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
5			Thieno[3,2-b]pyridin-7-ol, Ac de...	193	C9H7N2O2S	1000496-74-7	47



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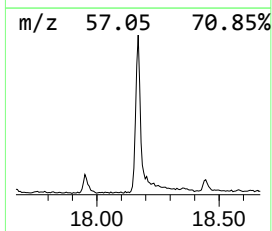
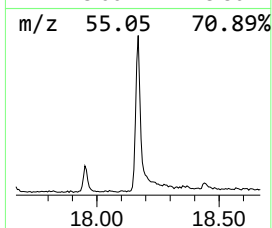
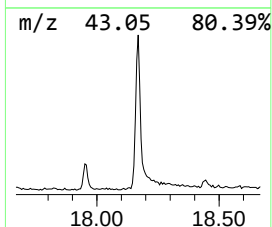
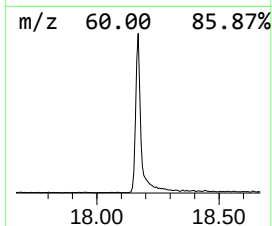
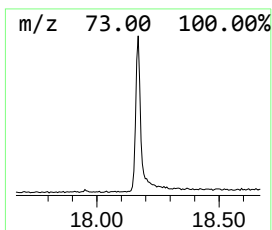
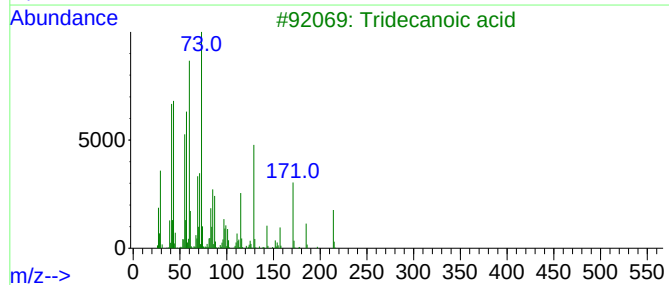
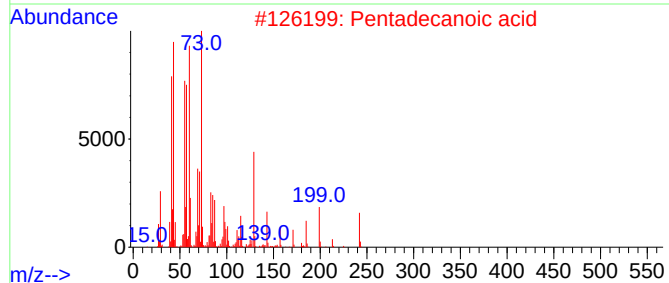
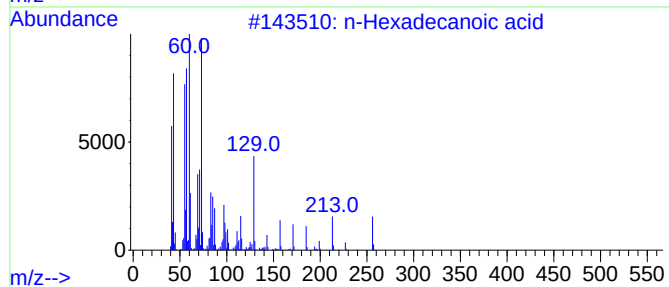
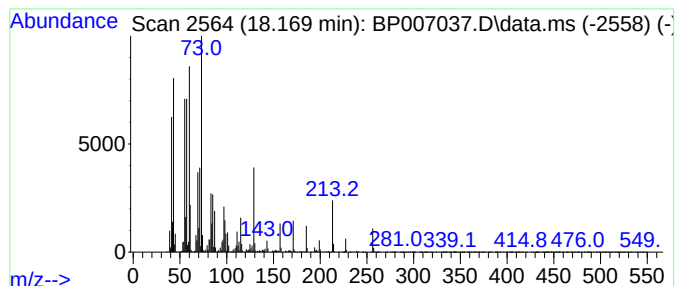
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	5.85 ng	1062140	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007037.D
Acq On : 17 Sep 2021 21:19
Operator : CG/JU
Sample : M3791-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

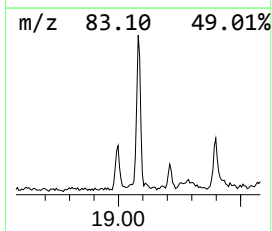
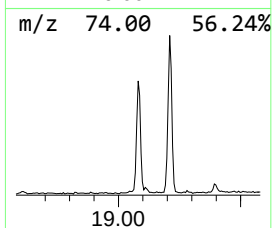
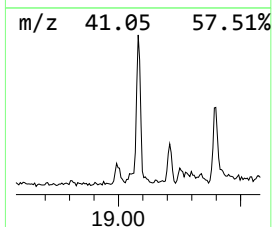
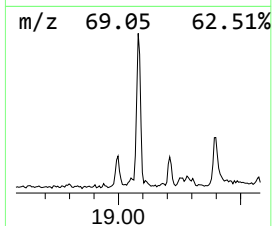
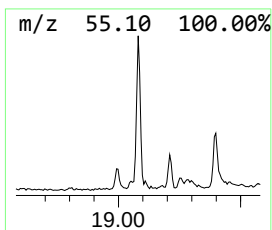
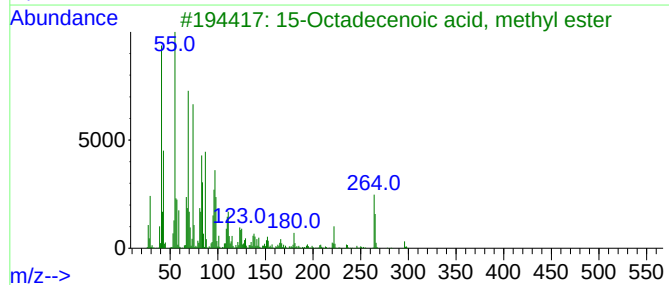
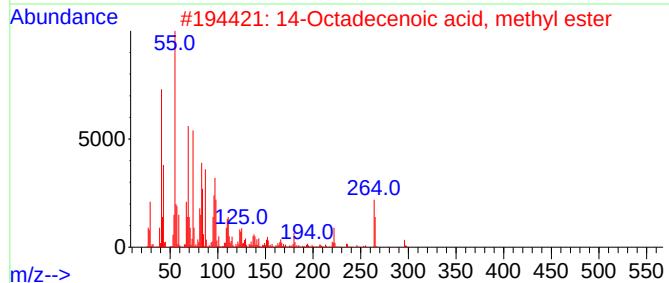
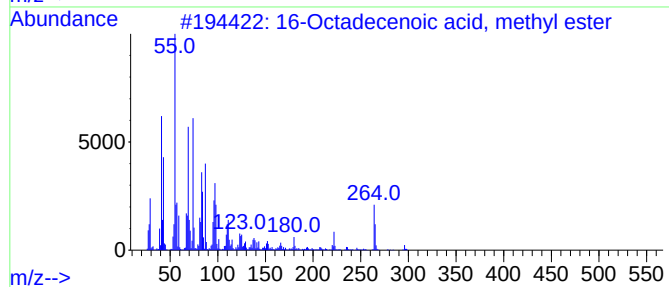
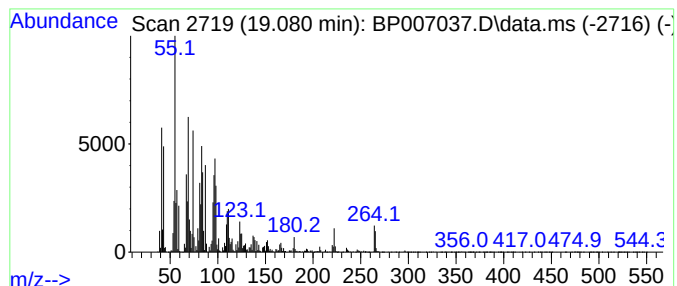
Instrument :
BNA_P
ClientSampleId :
SW-CB-03-(1.0)

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 8 16-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.080	2.95 ng	536167	Phenanthrene-d10	17.281	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
Data File : BP007037.D
Acq On : 17 Sep 2021 21:19
Operator : CG/JU
Sample : M3791-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-CB-03-(1.0)

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	2.8	ng	250405	1	7.905	1796840	20.0
Ethanol, 2-(2-b...	10.487	17.1	ng	2048980	2	10.704	2396010	20.0
2,4,7,9-Tetrame...	13.440	2.9	ng	447746	3	14.534	3120530	20.0
unknown15.486	15.486	2.3	ng	353968	3	14.534	3120530	20.0
2(3H)-Benzothia...	16.210	14.4	ng	2614360	4	17.281	3633730	20.0
n-Hexadecanoic ...	18.169	5.8	ng	1062140	4	17.281	3633730	20.0
16-Octadecenoic...	19.080	3.0	ng	536167	4	17.281	3633730	20.0