

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
 Data File : BP008329.D
 Acq On : 10 Dec 2021 01:04
 Operator : CG/JU
 Sample : M4967-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-7S

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-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.022	3	6	16	rVB	181766	208789	6.28%	1.180%
2	3.969	159	167	174	rVB	24424	39379	1.18%	0.223%
3	4.522	257	261	265	rVB	25188	33995	1.02%	0.192%
4	4.893	319	324	332	rBV	139632	203109	6.11%	1.148%
5	5.363	397	404	410	rBV	1046913	1621424	48.75%	9.164%
6	5.410	410	412	423	rVB	64302	114746	3.45%	0.649%
7	5.781	468	475	481	rVB	23503	34480	1.04%	0.195%
8	6.951	666	674	685	rBV	924140	1644099	49.43%	9.292%
9	7.763	805	812	820	rBV	235172	374059	11.25%	2.114%
10	8.928	1003	1010	1024	rBV	594168	1026275	30.86%	5.800%
11	10.563	1281	1288	1305	rBV	254348	471924	14.19%	2.667%
12	13.034	1700	1708	1727	rBV	1297098	2028458	60.99%	11.465%
13	14.328	1920	1928	1937	rBV2	20119	41769	1.26%	0.236%
14	14.422	1937	1944	1953	rBV	378894	614938	18.49%	3.476%
15	15.845	2181	2186	2192	rBV	77068	106583	3.20%	0.602%
16	15.922	2192	2199	2218	rBV	1014846	1670025	50.21%	9.439%
17	17.180	2407	2413	2422	rBV	479610	774103	23.27%	4.375%
18	17.310	2431	2435	2442	rVB5	26315	40342	1.21%	0.228%
19	17.845	2522	2526	2533	rVB6	17965	38135	1.15%	0.216%
20	18.080	2562	2566	2573	rBV2	83301	129707	3.90%	0.733%
21	18.980	2716	2719	2725	rVB3	25716	38417	1.16%	0.217%
22	19.757	2845	2851	2861	rVB	2654216	3325921	100.00%	18.798%
23	20.504	2975	2978	2981	rBV	60089	61062	1.84%	0.345%
24	21.004	3058	3063	3073	rBV	331183	540569	16.25%	3.055%
25	21.198	3093	3096	3101	rVB	135512	149148	4.48%	0.843%
26	21.292	3107	3112	3124	rBV	777840	1080076	32.47%	6.105%
27	22.174	3259	3262	3267	rVB	93879	111233	3.34%	0.629%
28	23.674	3511	3517	3529	rVB2	545910	1170200	35.18%	6.614%

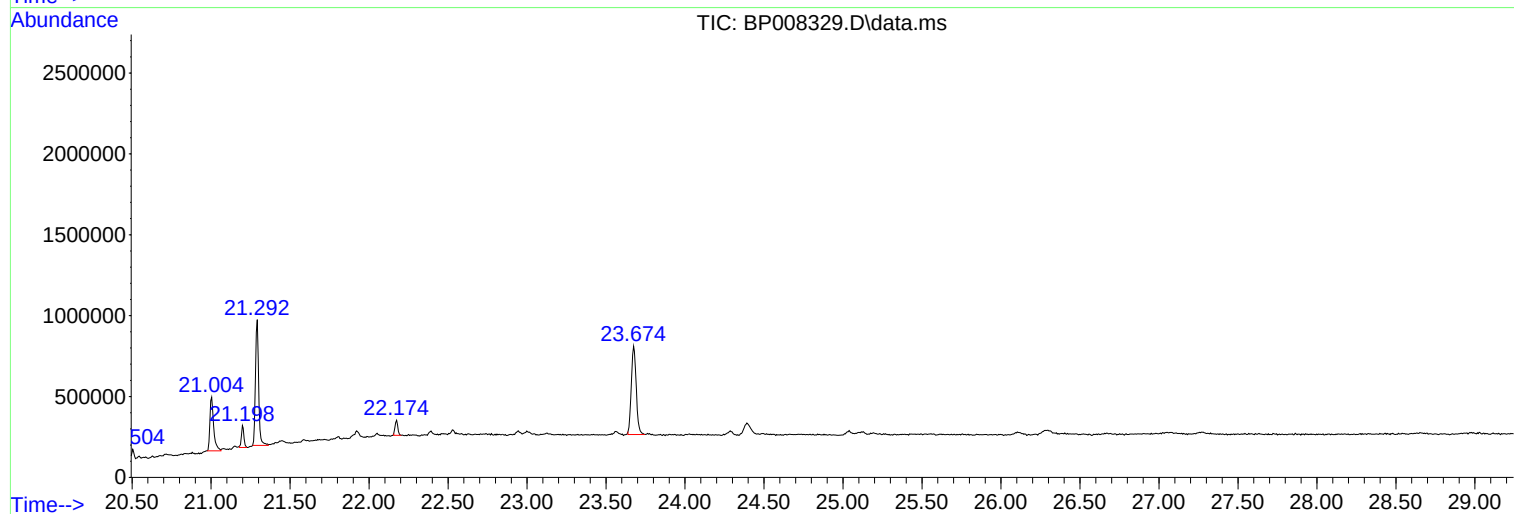
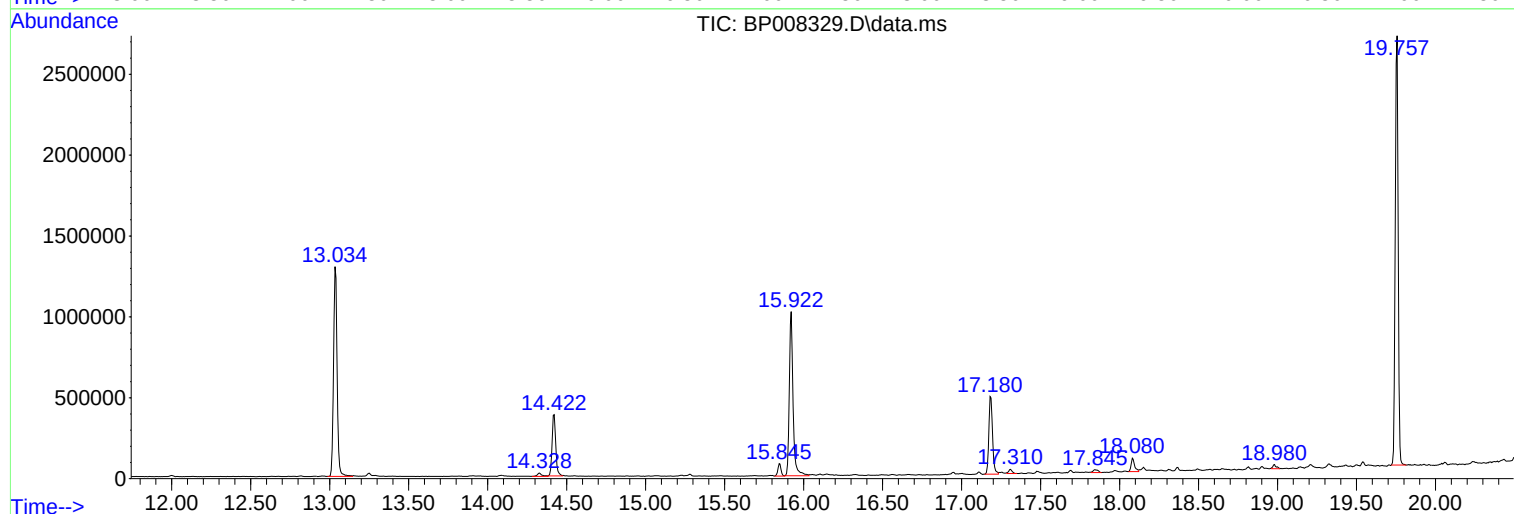
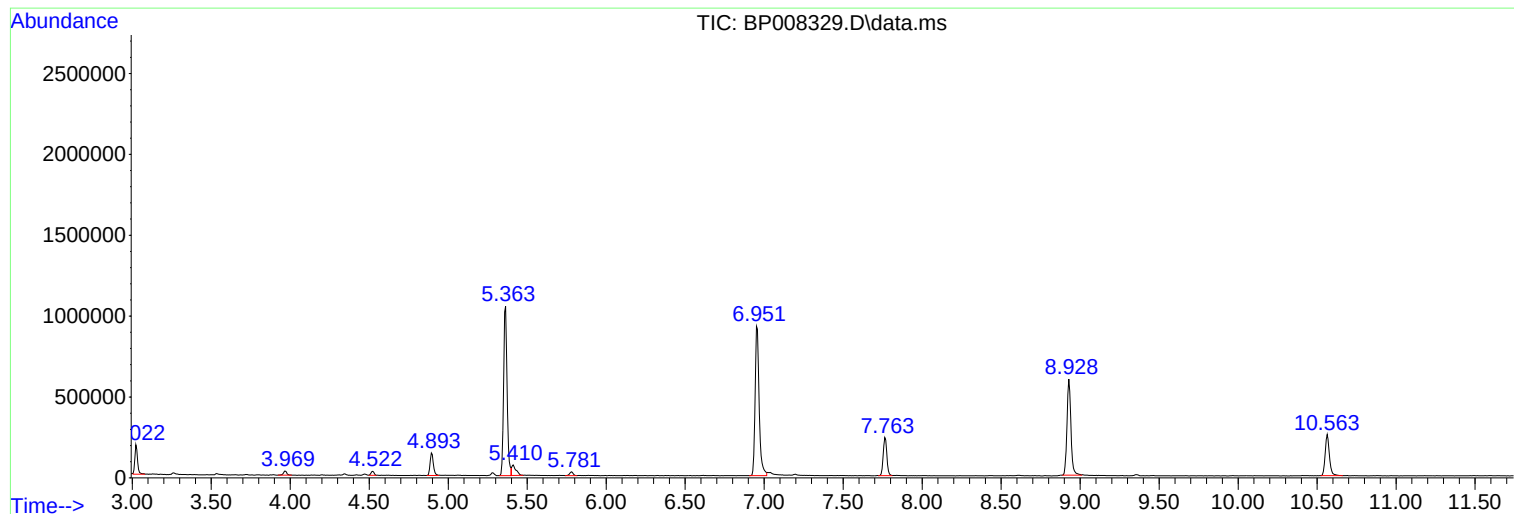
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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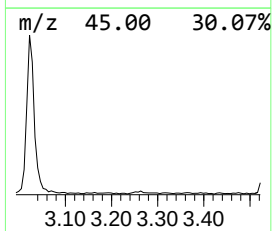
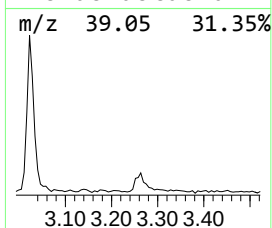
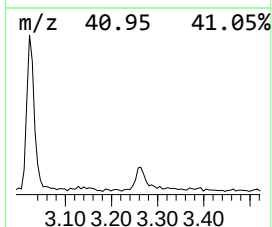
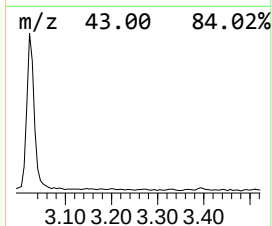
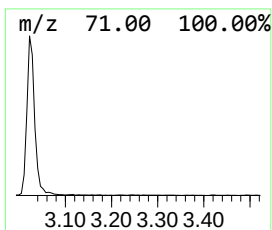
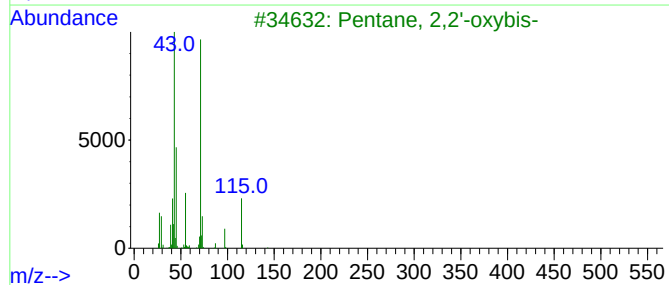
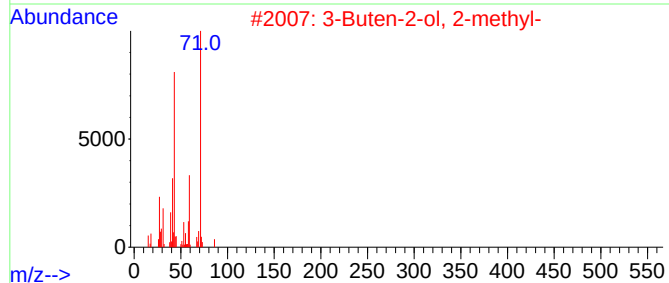
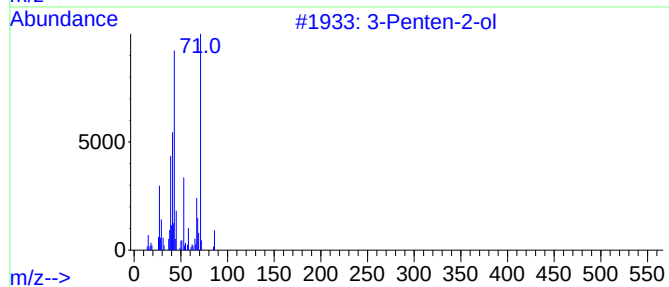
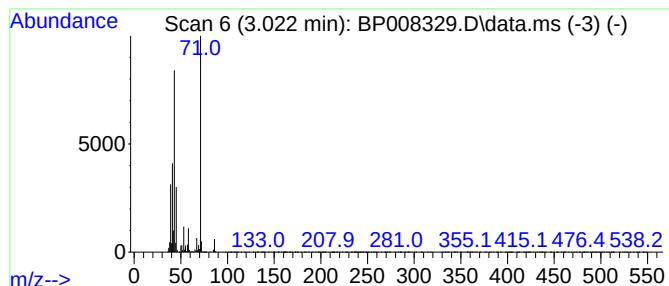
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.022	11.16 ng	208789	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-ol	86	C5H10O	001569-50-2	72
2			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
3			Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	64
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	56
5			Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53



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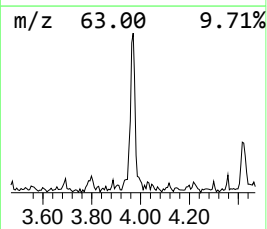
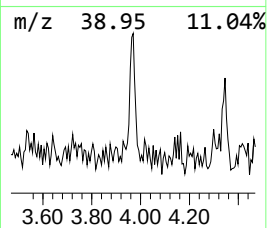
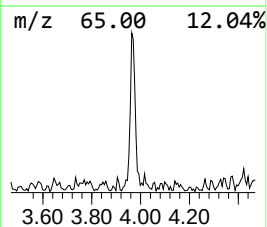
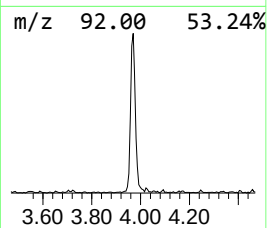
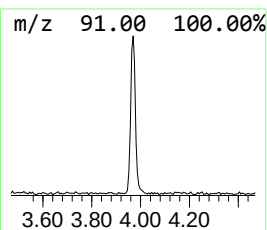
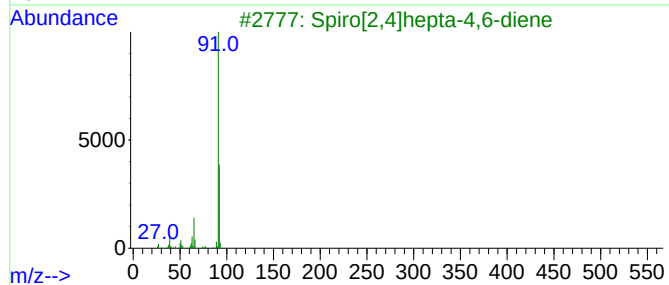
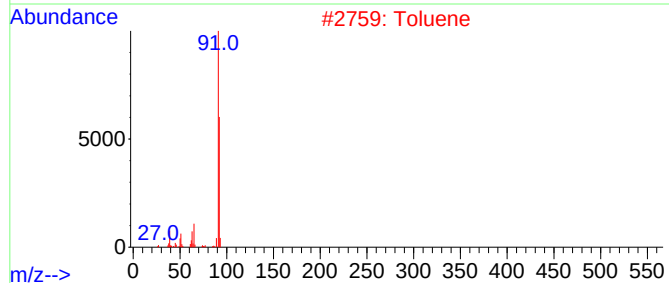
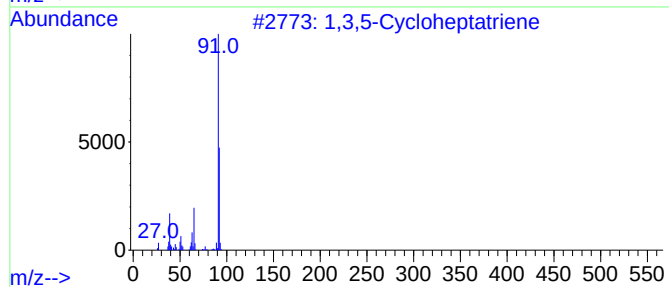
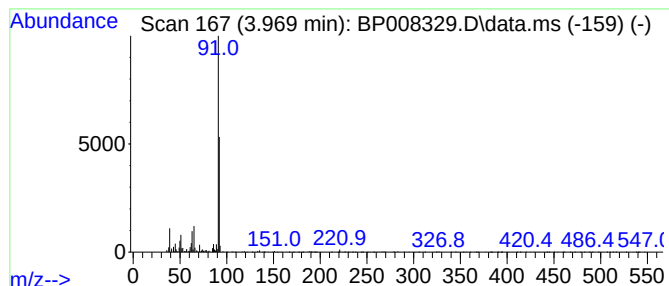
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.969	2.11 ng	39379	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
2			Toluene	92	C7H8	000108-88-3	90
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	83
4			Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	72
5			1,5-Heptadien-3-yne	92	C7H8	003511-27-1	64



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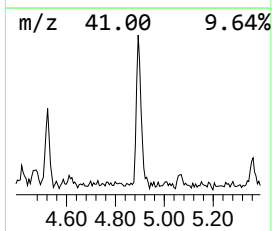
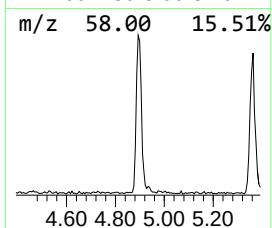
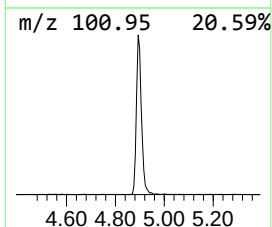
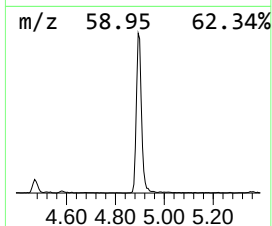
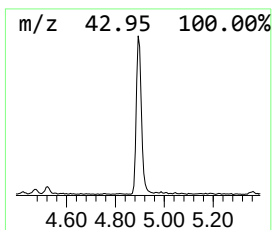
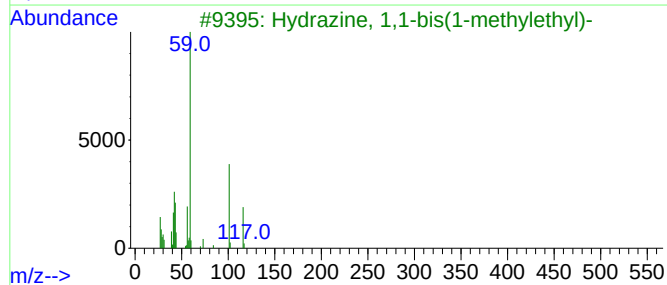
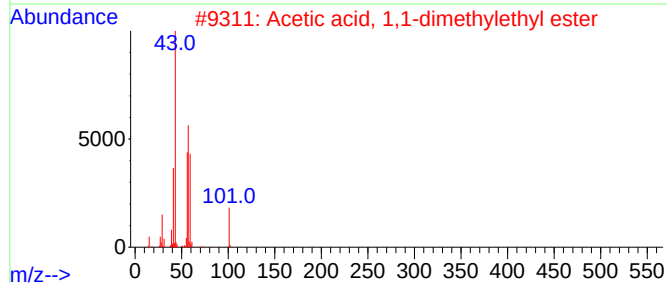
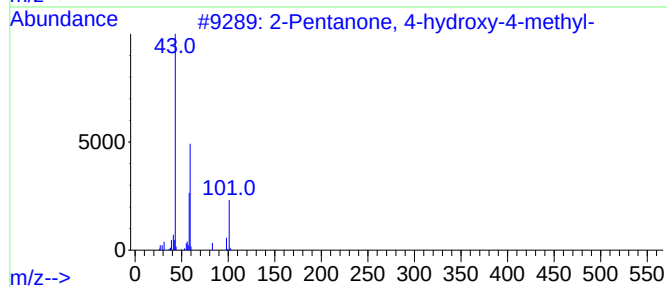
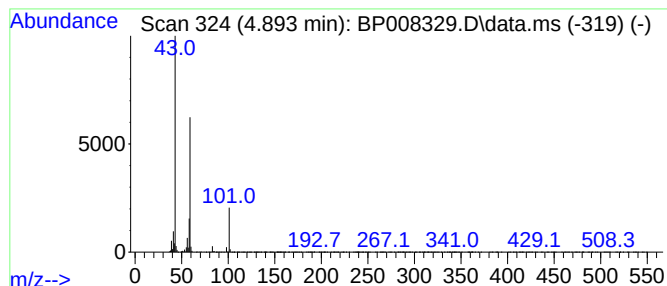
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	10.86 ng	203109	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			3-Hexanol	102	C6H14O	000623-37-0	28



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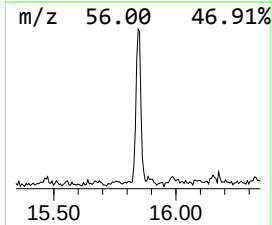
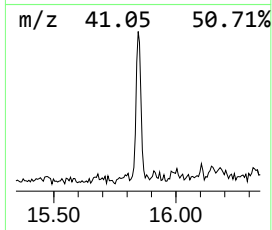
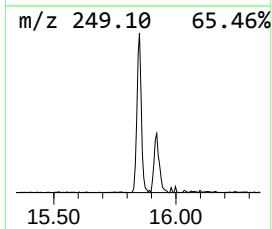
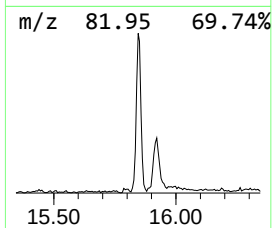
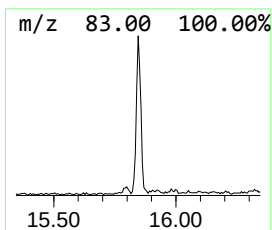
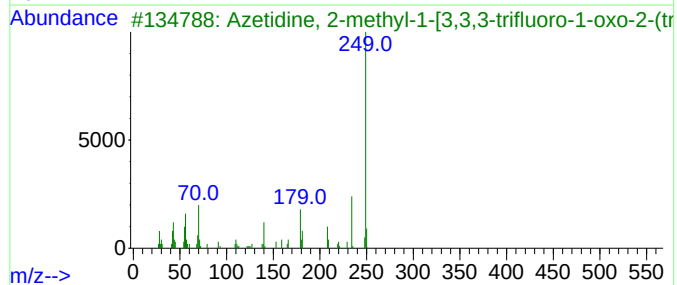
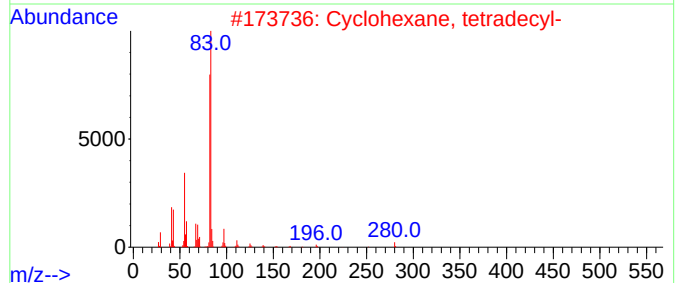
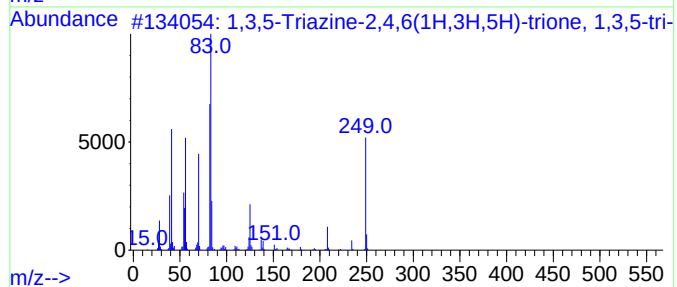
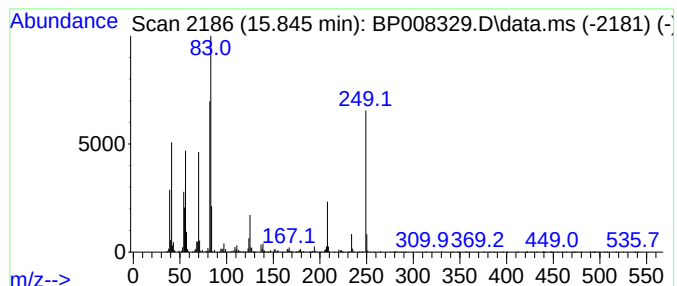
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Peak Number 4 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.845	2.75 ng	106583	Phenanthrene-d10	17.180	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	95
2	Cyclohexane, tetradecyl-	280	C20H40	001795-18-2	25
3	Azetidine, 2-methyl-1-[3,3,3-tri...	249	C8H9F6NO	050837-79-1	25
4	Cyclohexane, decyl-	224	C16H32	001795-16-0	25
5	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	25



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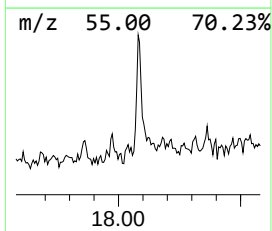
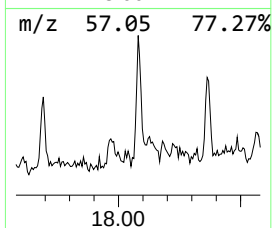
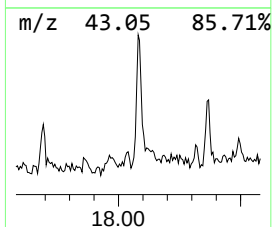
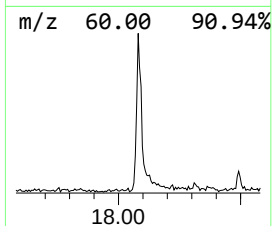
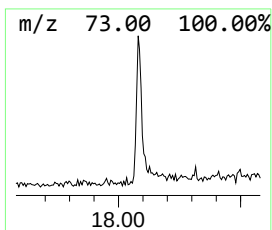
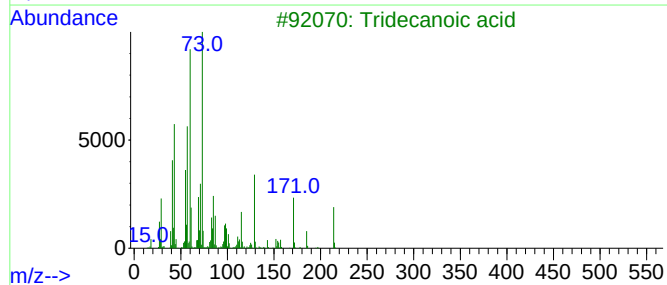
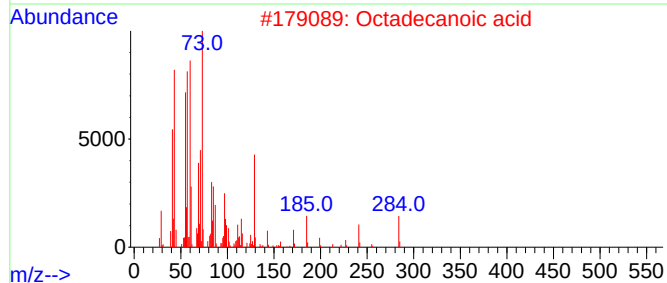
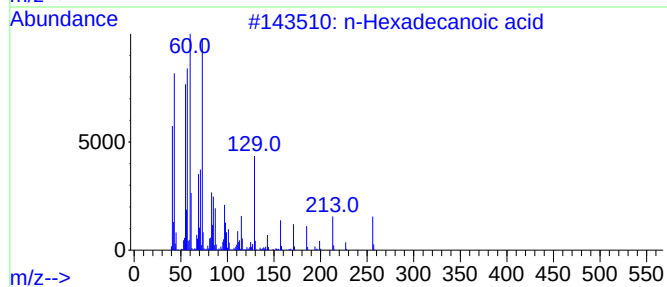
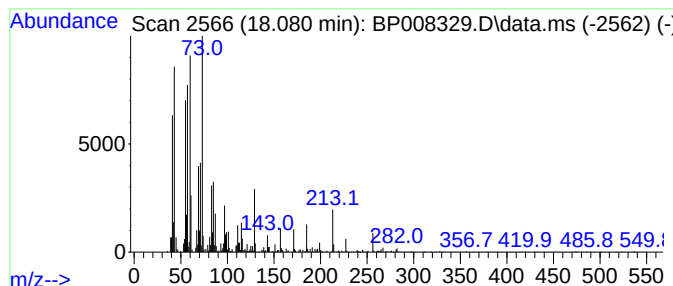
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.080	3.35 ng	129707	Phenanthrene-d10	17.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	64



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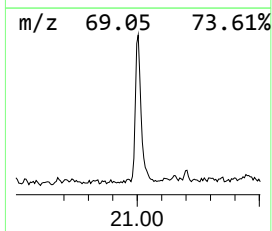
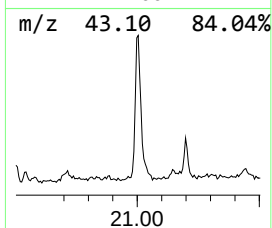
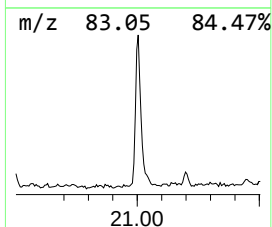
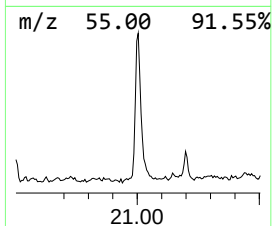
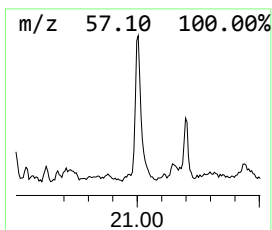
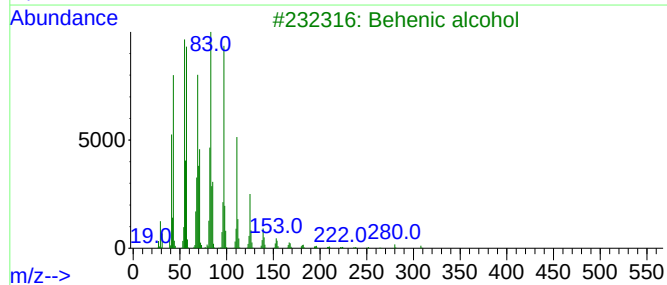
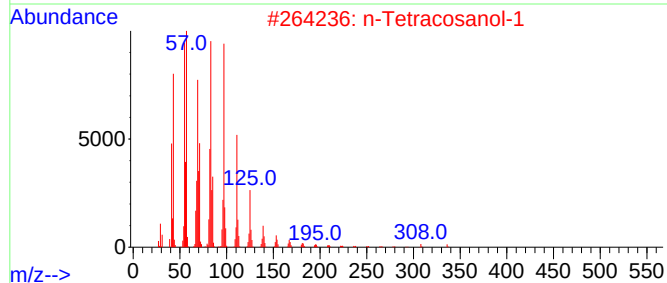
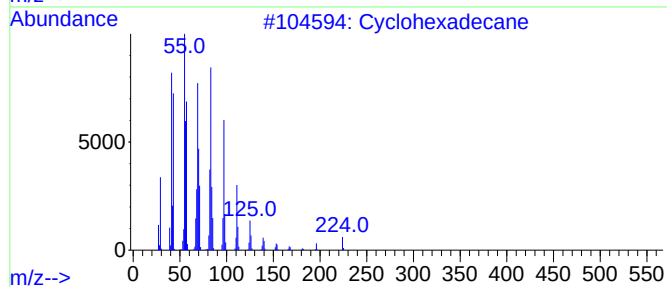
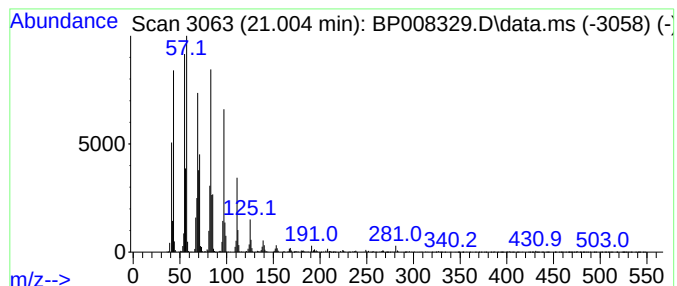
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.004	10.01 ng	540569	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
Data File : BP008329.D
Acq On : 10 Dec 2021 01:04
Operator : CG/JU
Sample : M4967-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-7S

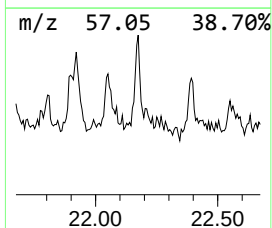
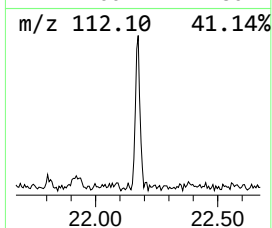
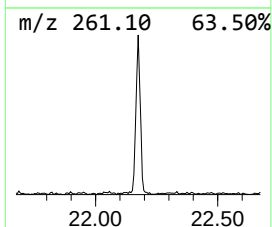
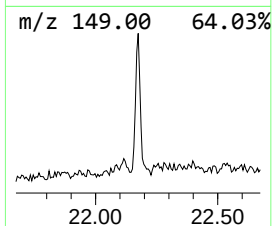
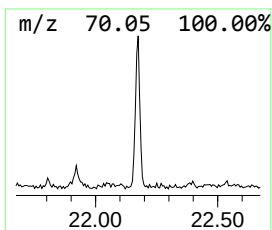
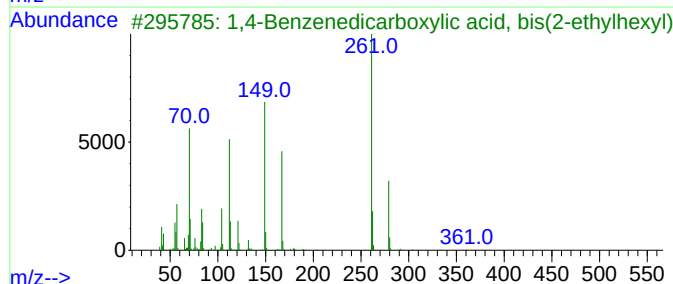
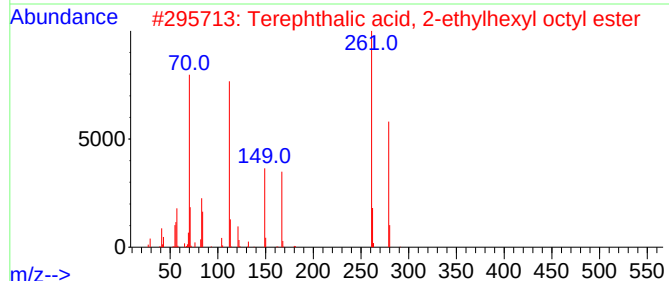
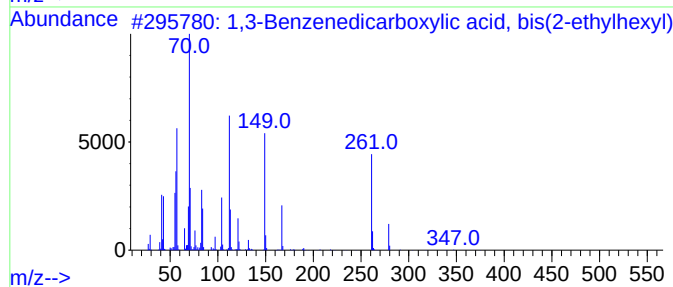
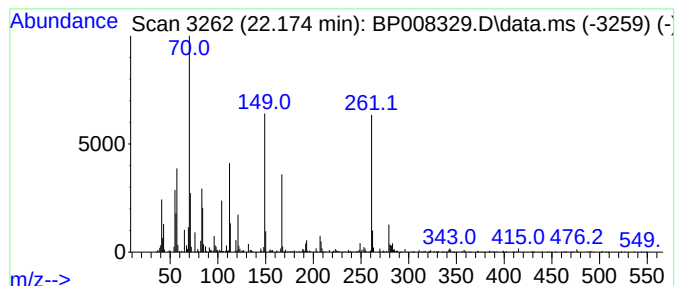
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.174	2.06 ng	111233	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	83
2			Terephthalic acid, 2-ethylhexyl ...	390	C24H3804	1000324-00-5	53
3			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	50
4			Terephthalic acid, 3-hexyl octyl...	362	C22H3404	1000356-23-1	38
5			Isophthalic acid, di(4-octyl) ester	390	C24H3804	1000344-04-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
Data File : BP008329.D
Acq On : 10 Dec 2021 01:04
Operator : CG/JU
Sample : M4967-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-7S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
3-Penten-2-ol	3.022	11.2	ng	208789	1	7.763	374059	20.0
1,3,5-Cyclohept...	3.969	2.1	ng	39379	1	7.763	374059	20.0
2-Pentanone, 4-...	4.893	10.9	ng	203109	1	7.763	374059	20.0
1,3,5-Triazine-...	15.845	2.8	ng	106583	4	17.180	774103	20.0
n-Hexadecanoic ...	18.080	3.4	ng	129707	4	17.180	774103	20.0
Cyclohexadecane	21.004	10.0	ng	540569	5	21.292	1080080	20.0
1,3-Benzenedica...	22.174	2.1	ng	111233	5	21.292	1080080	20.0