

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
 Data File : BP013615.D
 Acq On : 27 Jan 2023 13:32
 Operator : CG/JU
 Sample : 01221-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-1-0118

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-BP012623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013615.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.223	3	6	27	rVB	3937299	4545160	45.23%	8.317%
2	5.211	338	344	354	rBV	434614	618741	6.16%	1.132%
3	5.681	417	424	435	rBV	1468439	2161895	21.52%	3.956%
4	7.293	691	698	707	rBV	826864	1304219	12.98%	2.387%
5	8.152	837	844	851	rBV	760098	1201475	11.96%	2.199%
6	9.328	1036	1044	1053	rBV	2111345	3385794	33.70%	6.195%
7	10.987	1318	1326	1339	rBV	916837	1598517	15.91%	2.925%
8	13.416	1732	1739	1753	rBV	5629312	8315071	82.75%	15.215%
9	14.793	1966	1973	1984	rVB	1271712	1950371	19.41%	3.569%
10	16.145	2198	2203	2211	rVB	201819	308235	3.07%	0.564%
11	16.275	2219	2225	2234	rBV	3828007	5665995	56.39%	10.368%
12	16.604	2265	2281	2296	rBV2	783692	2452501	24.41%	4.488%
13	17.187	2374	2380	2390	rBV	914488	1294640	12.88%	2.369%
14	17.545	2435	2441	2448	rBV	1543643	2177486	21.67%	3.984%
15	18.404	2582	2587	2596	rBV	732562	1160054	11.54%	2.123%
16	19.628	2791	2795	2808	rBV	324522	482678	4.80%	0.883%
17	20.075	2866	2871	2881	rVB	7759632	10048154	100.00%	18.387%
18	21.298	3075	3079	3090	rBV	321767	488641	4.86%	0.894%
19	21.627	3129	3135	3139	rBV	1896797	2607492	25.95%	4.771%
20	24.216	3568	3575	3584	rVB2	1323651	2882363	28.69%	5.274%

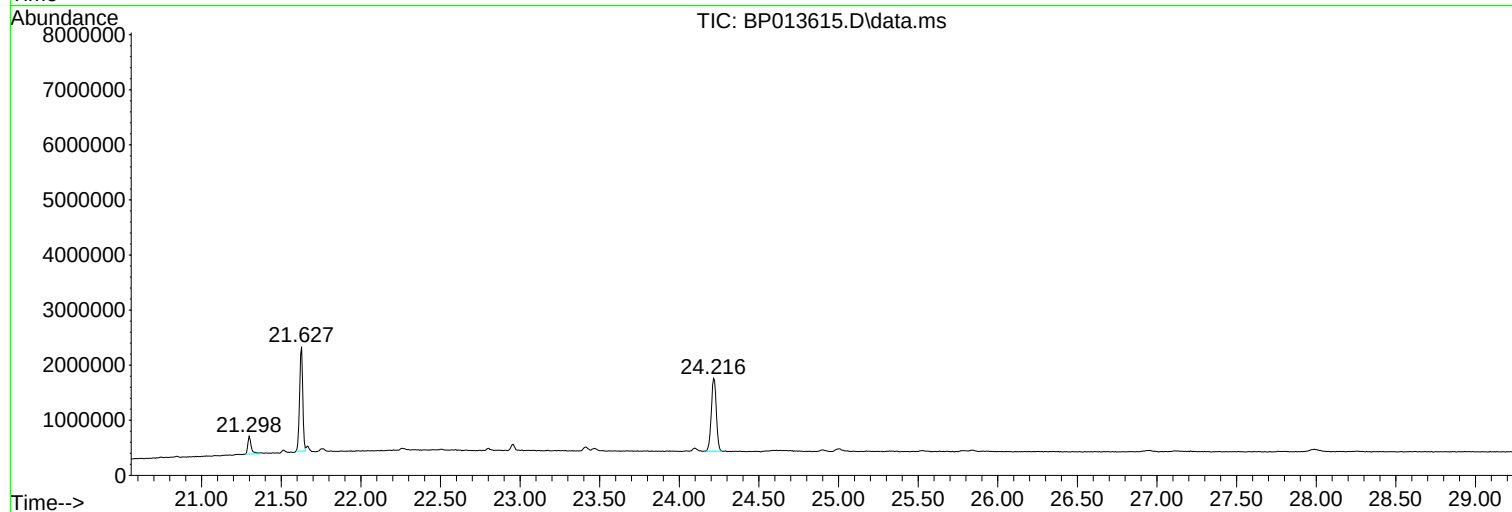
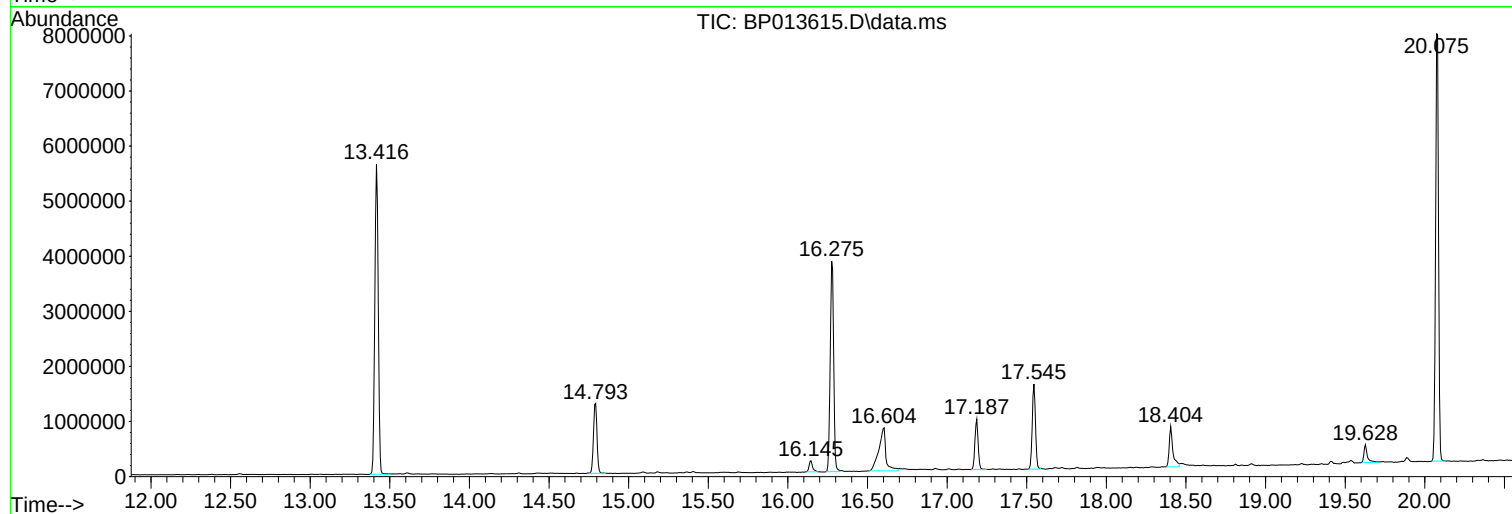
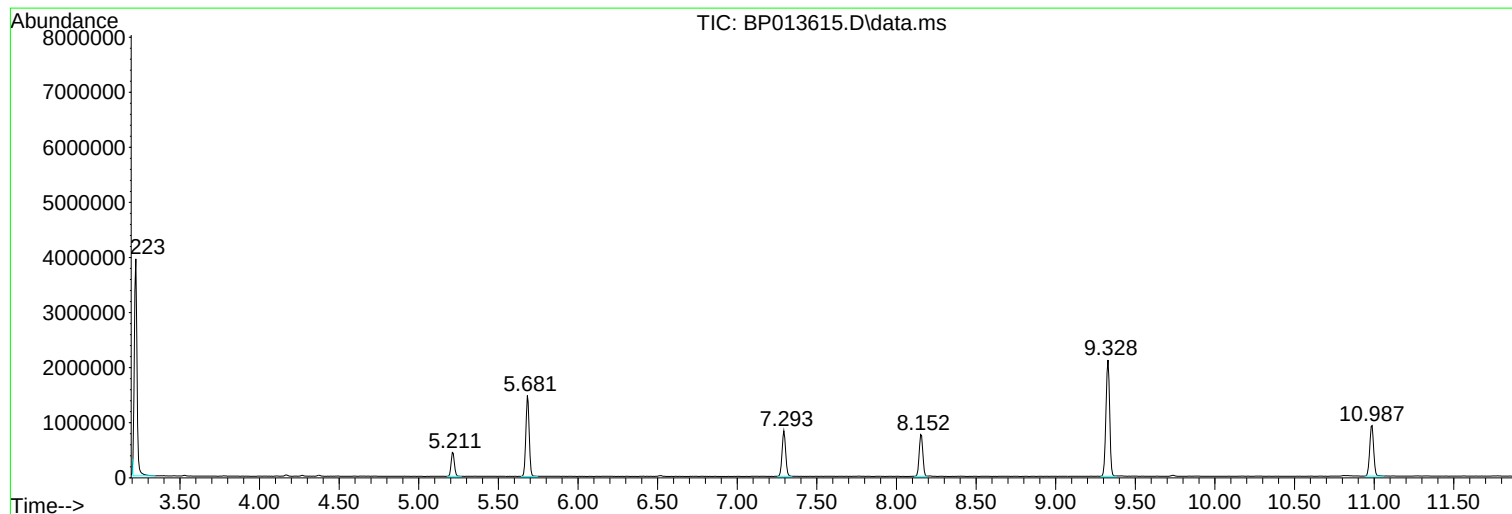
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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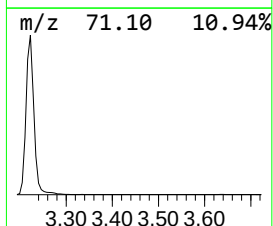
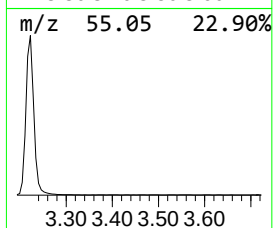
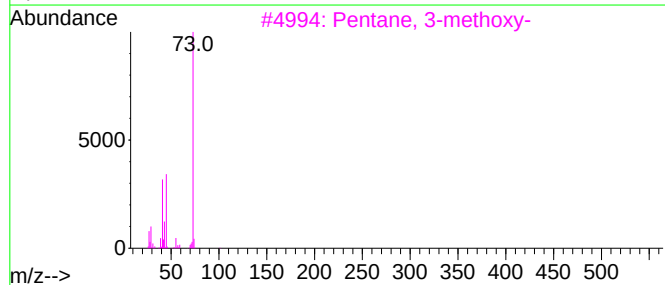
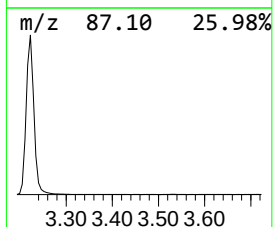
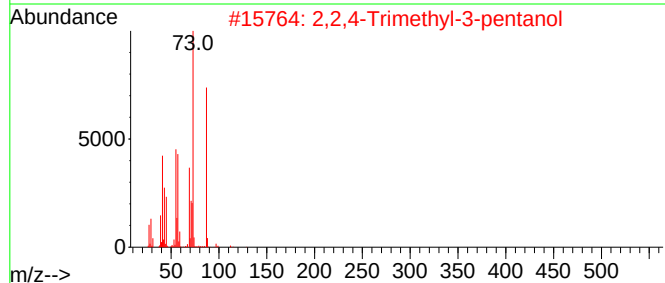
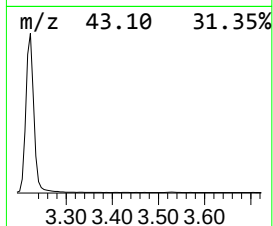
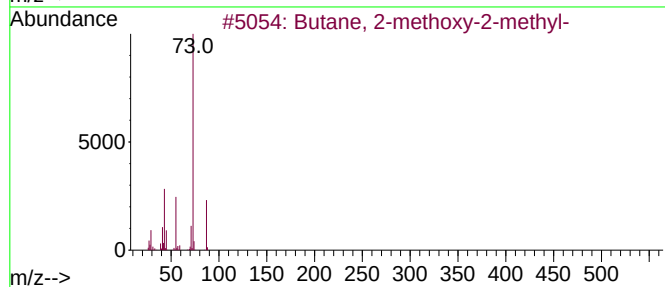
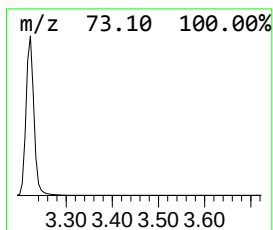
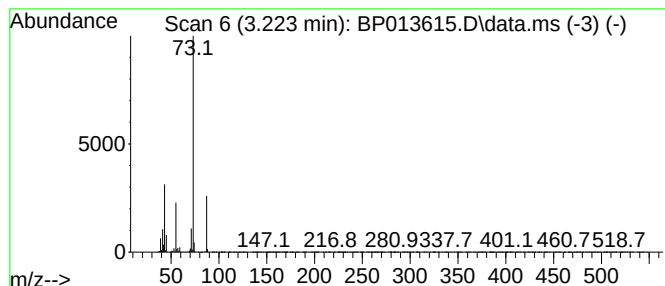
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.223	75.66 ng	4545160	1,4-Dichlorobenzene-d4	8.152

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	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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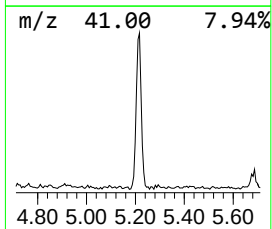
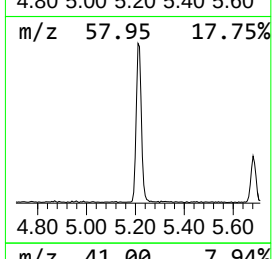
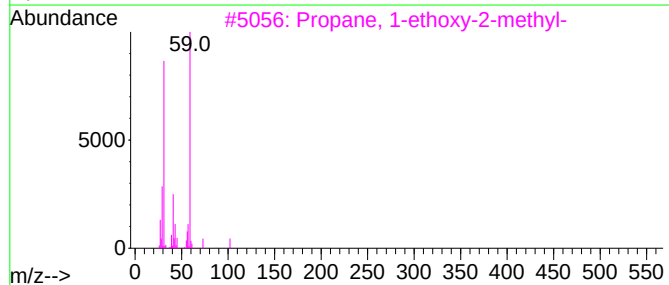
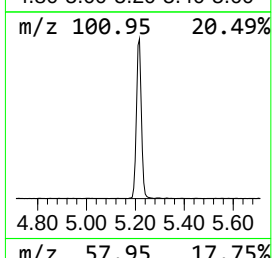
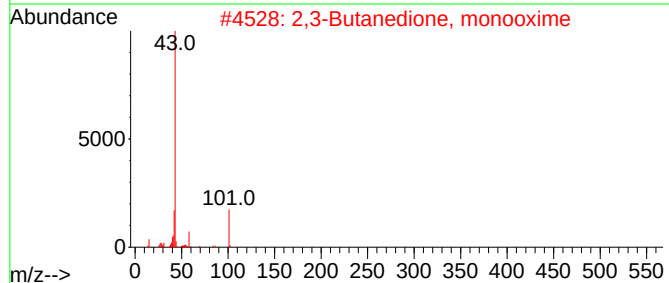
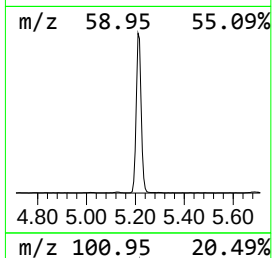
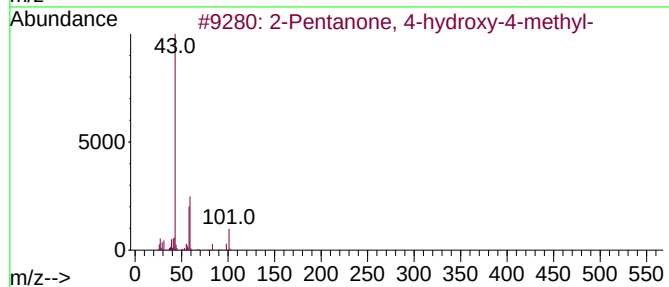
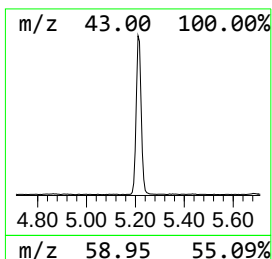
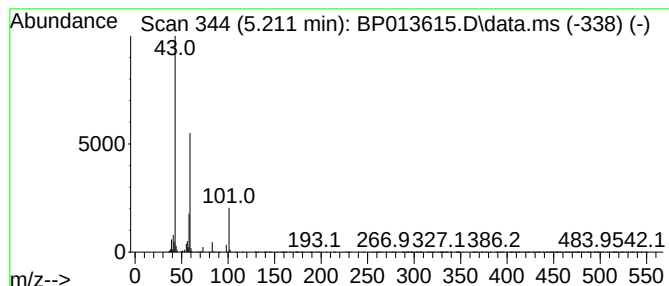
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.211	10.30 ng	618741	1,4-Dichlorobenzene-d4	8.152

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4			Hexanamide	115	C6H13NO	000628-02-4	12
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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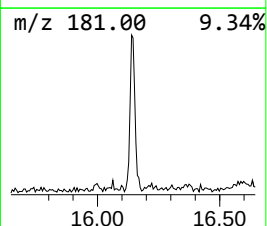
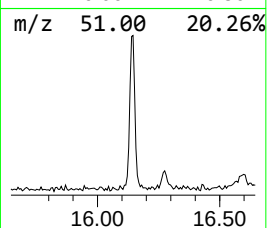
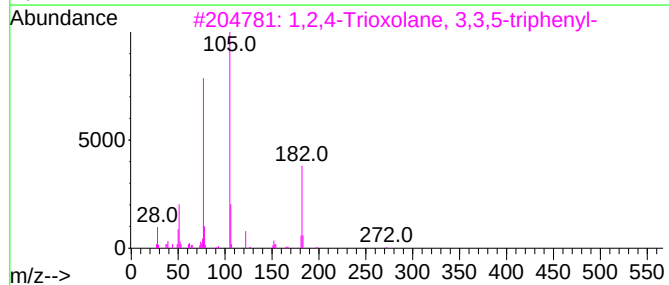
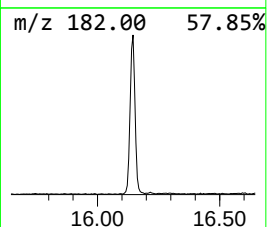
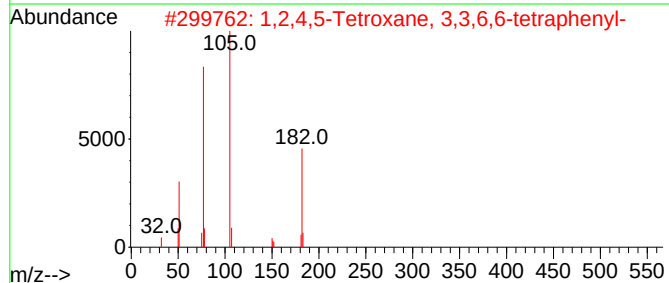
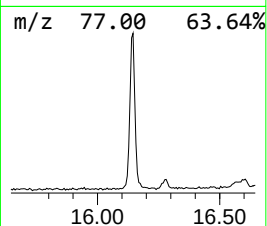
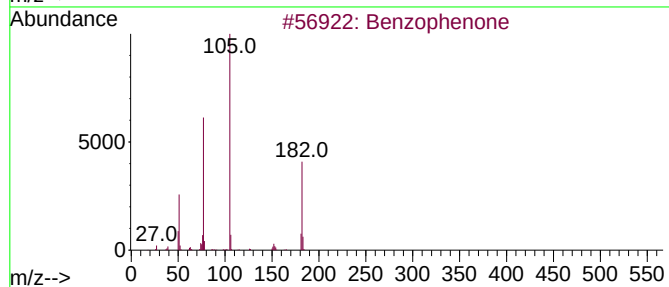
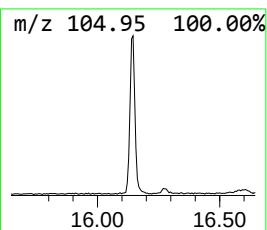
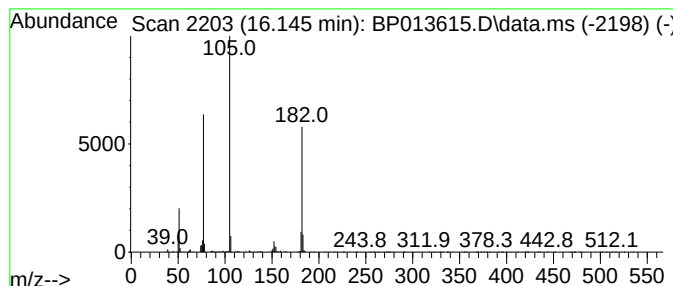
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	3.16 ng	308235	Acenaphthene-d10	14.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	64
3			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50
4			Azobenzene	182	C12H10N2	000103-33-3	42
5			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	38



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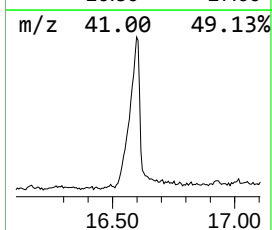
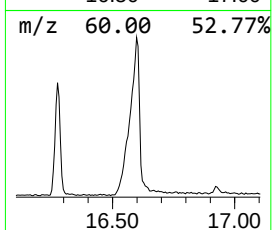
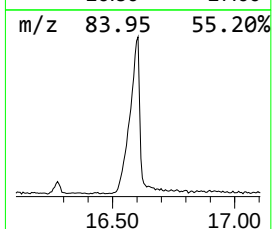
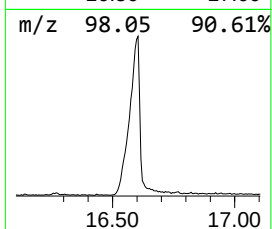
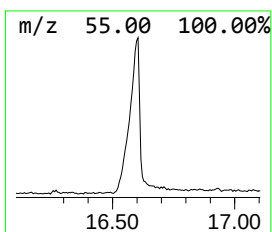
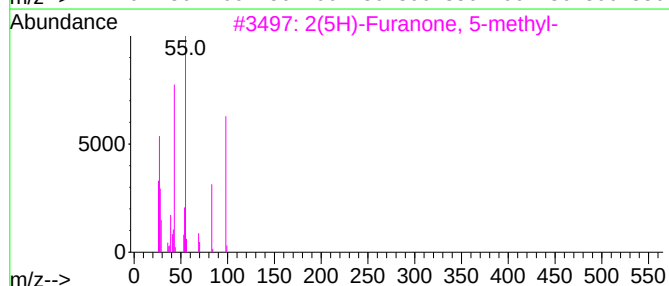
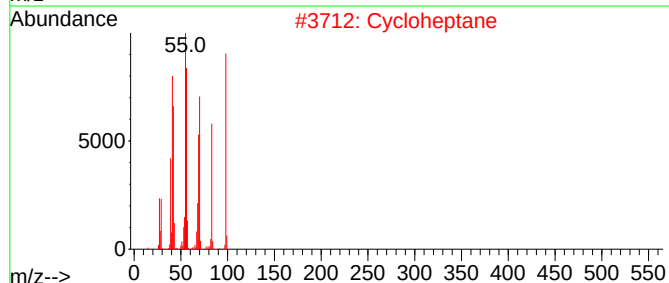
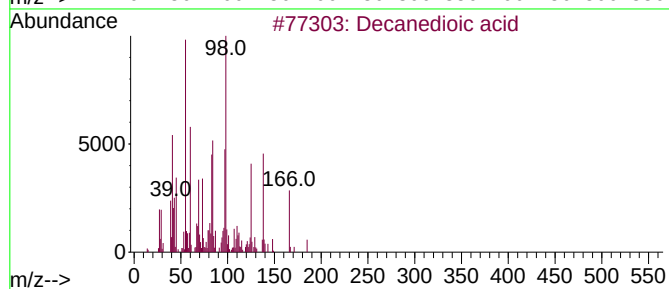
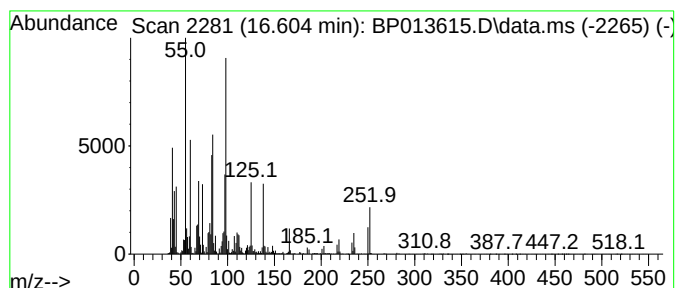
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Peak Number 4 Decanedioic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.604	22.53 ng	2452500	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanedioic acid	202	C10H18O4	000111-20-6	91
2			Cycloheptane	98	C7H14	000291-64-5	27
3			2(5H)-Furanone, 5-methyl-	98	C5H6O2	000591-11-7	27
4			.beta.-Piperidinopropiophenone	217	C14H19NO	000073-63-2	25
5			N-Chloro-16-iso-tetrahydrosolaso...	451	C27H46ClNO2	1000256-11-2	22



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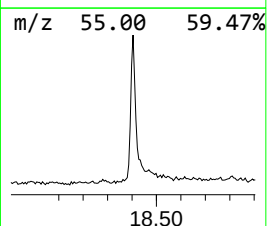
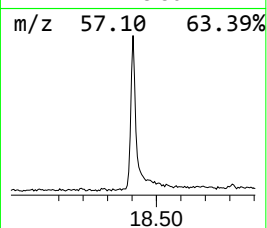
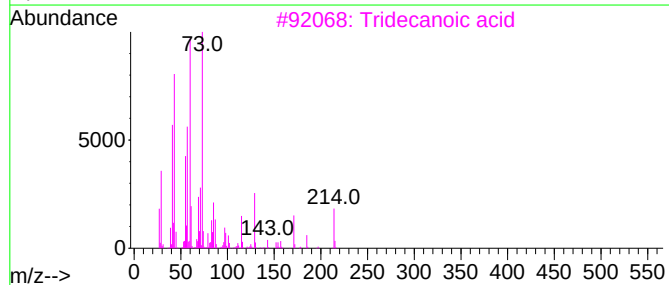
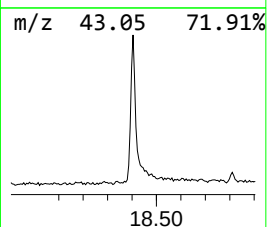
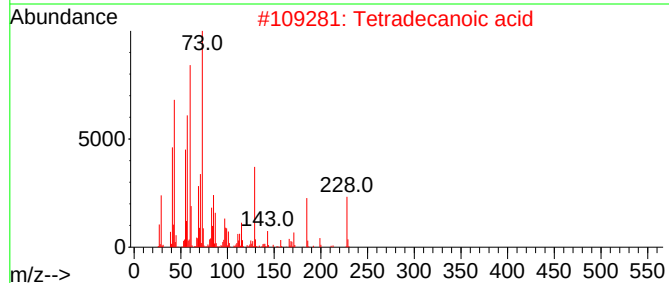
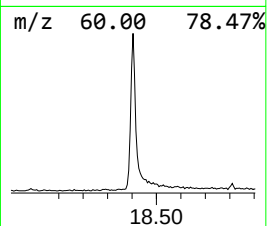
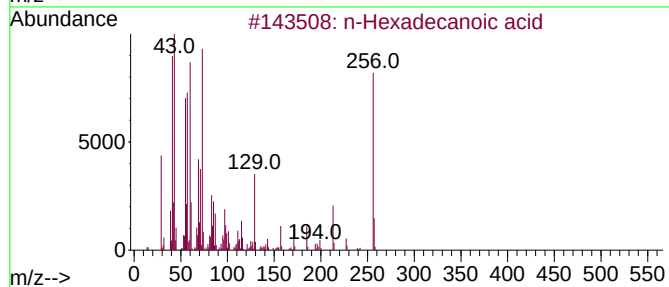
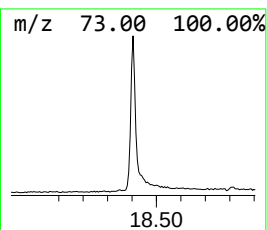
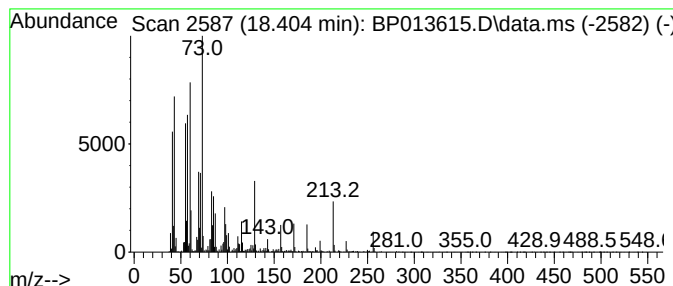
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.404	10.65 ng	1160050	Phenanthrene-d10	17.545

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			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	43



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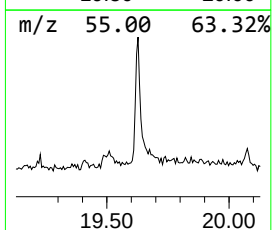
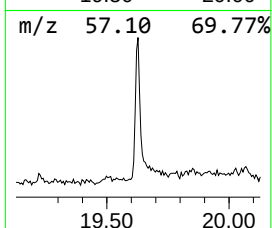
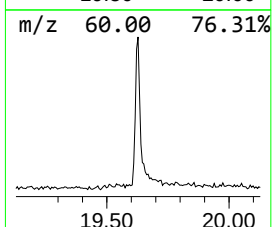
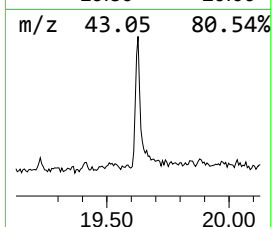
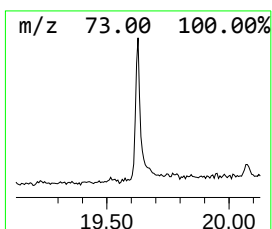
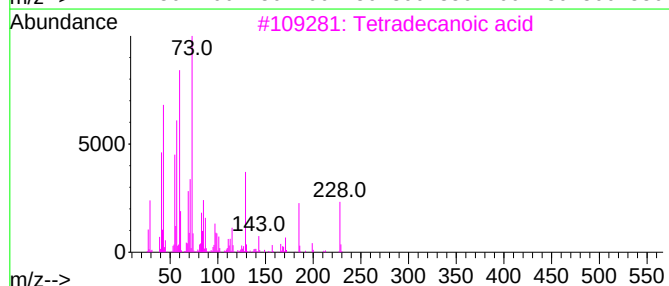
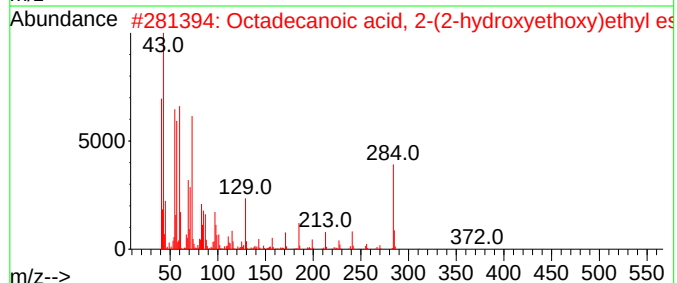
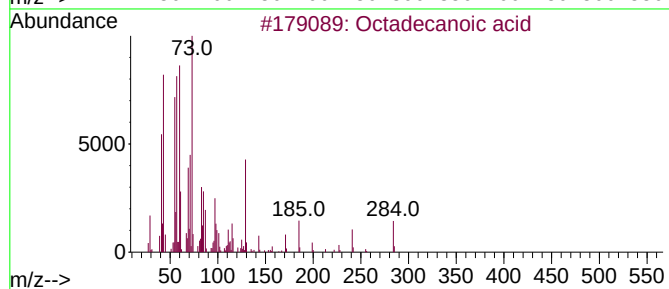
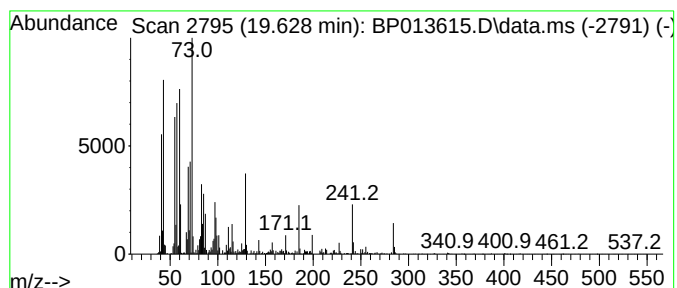
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.628	3.70 ng	482678	Chrysene-d12	21.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
Data File : BP013615.D
Acq On : 27 Jan 2023 13:32
Operator : CG/JU
Sample : 01221-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

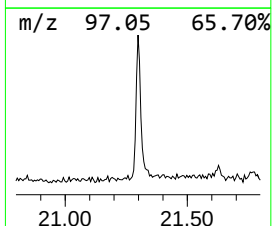
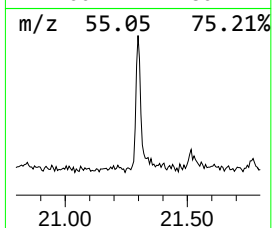
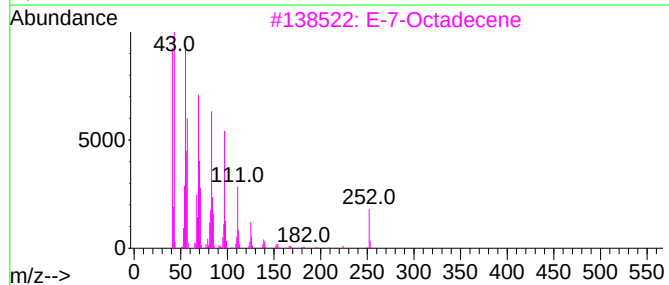
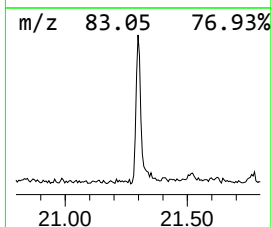
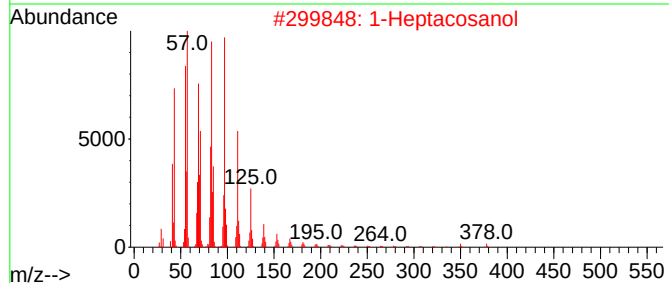
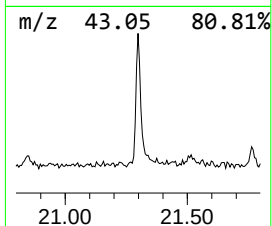
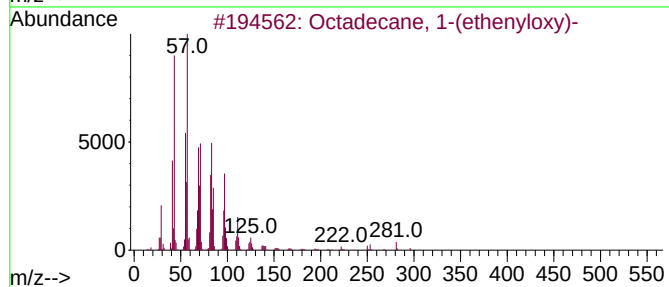
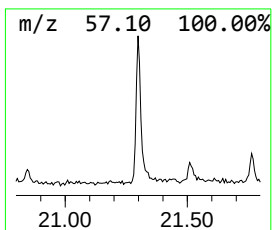
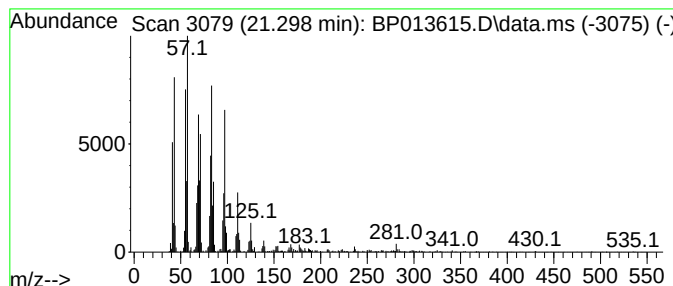
Instrument :
BNA_P
ClientSampleId :
MW-1-0118

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane, 1-(ethenyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.298	3.75 ng	488641	Chrysene-d12	21.628	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	E-7-Octadecene	252	C18H36	1000130-92-0	92
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
Data File : BP013615.D
Acq On : 27 Jan 2023 13:32
Operator : CG/JU
Sample : 01221-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1-0118

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.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
Butane, 2-metho...	3.223	75.7	ng	4545160	1	8.152	1201480	20.0
2-Pentanone, 4-...	5.211	10.3	ng	618741	1	8.152	1201480	20.0
Benzophenone	16.145	3.2	ng	308235	3	14.787	1950370	20.0
Decanedioic acid	16.604	22.5	ng	2452500	4	17.545	2177490	20.0
n-Hexadecanoic ...	18.404	10.7	ng	1160050	4	17.545	2177490	20.0
Octadecanoic acid	19.628	3.7	ng	482678	5	21.628	2607490	20.0
Octadecane, 1-(...	21.298	3.8	ng	488641	5	21.628	2607490	20.0