

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052623\
 Data File : BP015311.D
 Acq On : 26 May 2023 16:17
 Operator : CG/JU
 Sample : 02908-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TWP02

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-BP052423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP015311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.158	330	335	343	rVB	100140	138888	1.58%	0.330%
2	5.634	409	416	427	rBV	1475013	2131212	24.27%	5.059%
3	7.258	685	692	702	rVB	889144	1380828	15.73%	3.278%
4	8.105	829	836	844	rBV	511494	795438	9.06%	1.888%
5	9.281	1028	1036	1045	rBV	1641499	2716987	30.94%	6.450%
6	10.934	1310	1317	1325	rVB	616414	1019469	11.61%	2.420%
7	13.375	1725	1732	1739	rBV	3841100	5542332	63.12%	13.157%
8	14.745	1959	1965	1974	rBV	913602	1291731	14.71%	3.067%
9	15.140	2028	2032	2039	rVB	97617	138709	1.58%	0.329%
10	16.004	2171	2179	2187	rVB	111576	307658	3.50%	0.730%
11	16.104	2190	2196	2201	rVB	342712	481874	5.49%	1.144%
12	16.234	2212	2218	2226	rBV	2981227	4391476	50.01%	10.425%
13	16.881	2323	2328	2338	rBV3	136584	307152	3.50%	0.729%
14	17.498	2428	2433	2439	rBV	1089994	1596568	18.18%	3.790%
15	18.363	2573	2580	2591	rBV	2156281	3202374	36.47%	7.602%
16	18.639	2623	2627	2631	rBV	225837	321892	3.67%	0.764%
17	18.692	2631	2636	2647	rVB	389415	706416	8.04%	1.677%
18	18.880	2665	2668	2674	rVB2	72151	115651	1.32%	0.275%
19	19.445	2761	2764	2766	rBV2	80541	99689	1.14%	0.237%
20	19.586	2783	2788	2807	rVB	1230206	1778978	20.26%	4.223%
21	20.039	2859	2865	2870	rBV	7108774	8781041	100.00%	20.846%
22	20.322	2910	2913	2919	rVB3	85930	119757	1.36%	0.284%
23	20.798	2991	2994	2998	rVB	110694	129864	1.48%	0.308%
24	21.263	3069	3073	3081	rBV4	183432	294954	3.36%	0.700%
25	21.580	3122	3127	3132	rBV	1527390	2034841	23.17%	4.831%
26	24.127	3554	3560	3571	rVB	1034141	2297736	26.17%	5.455%

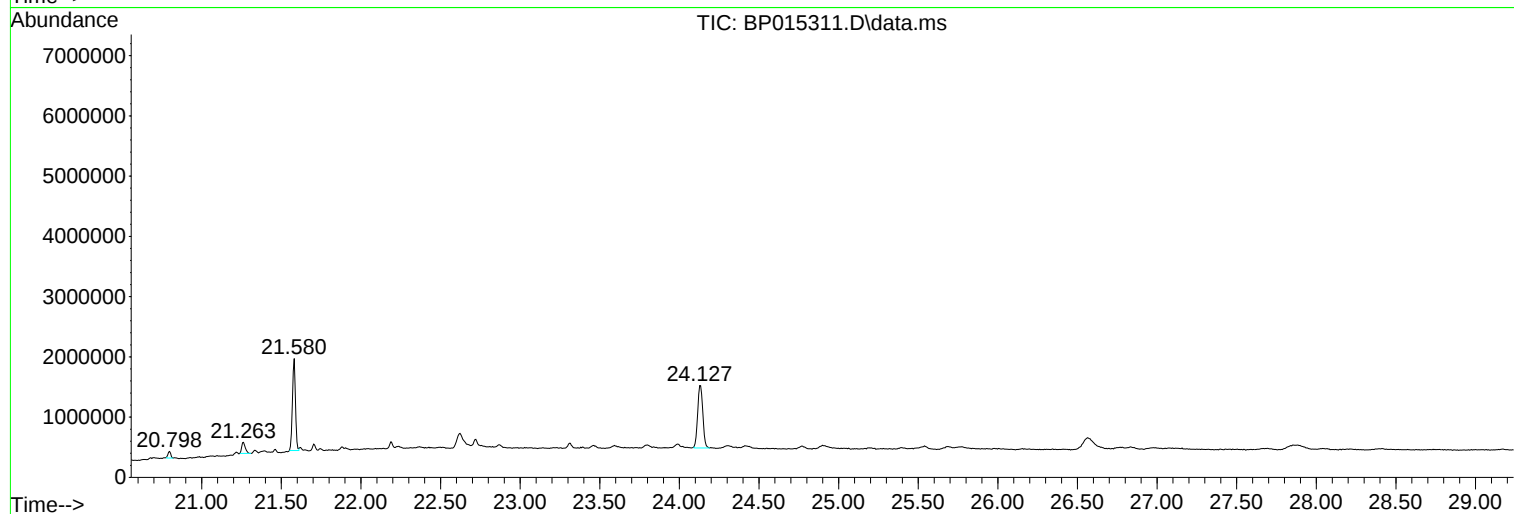
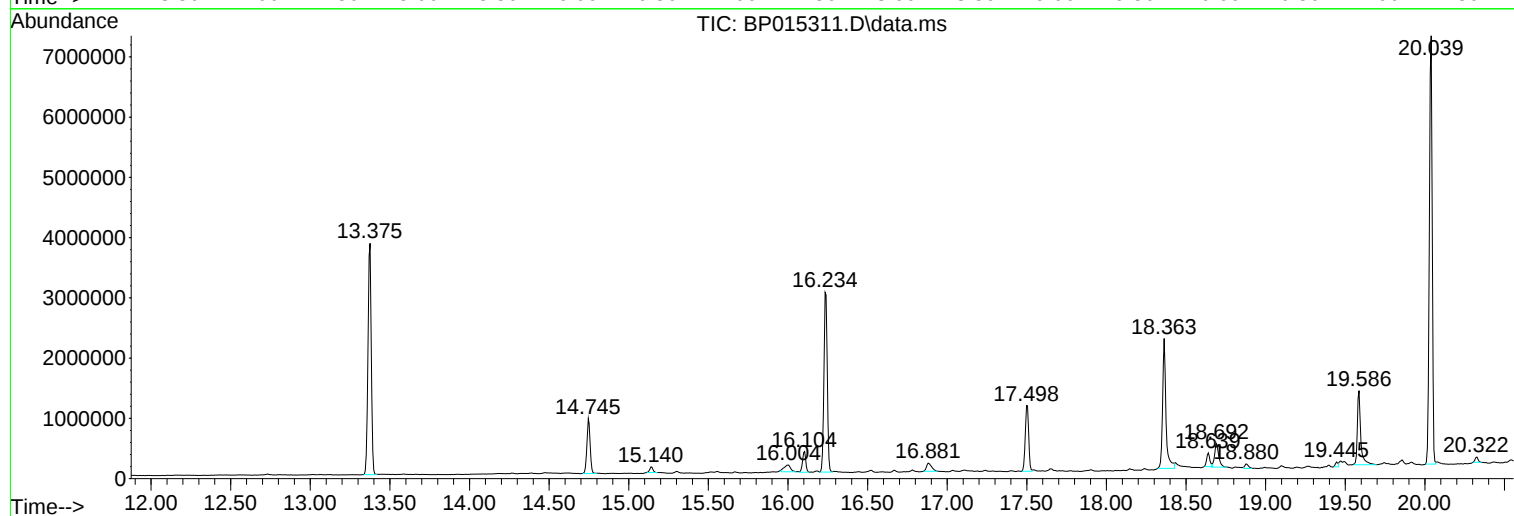
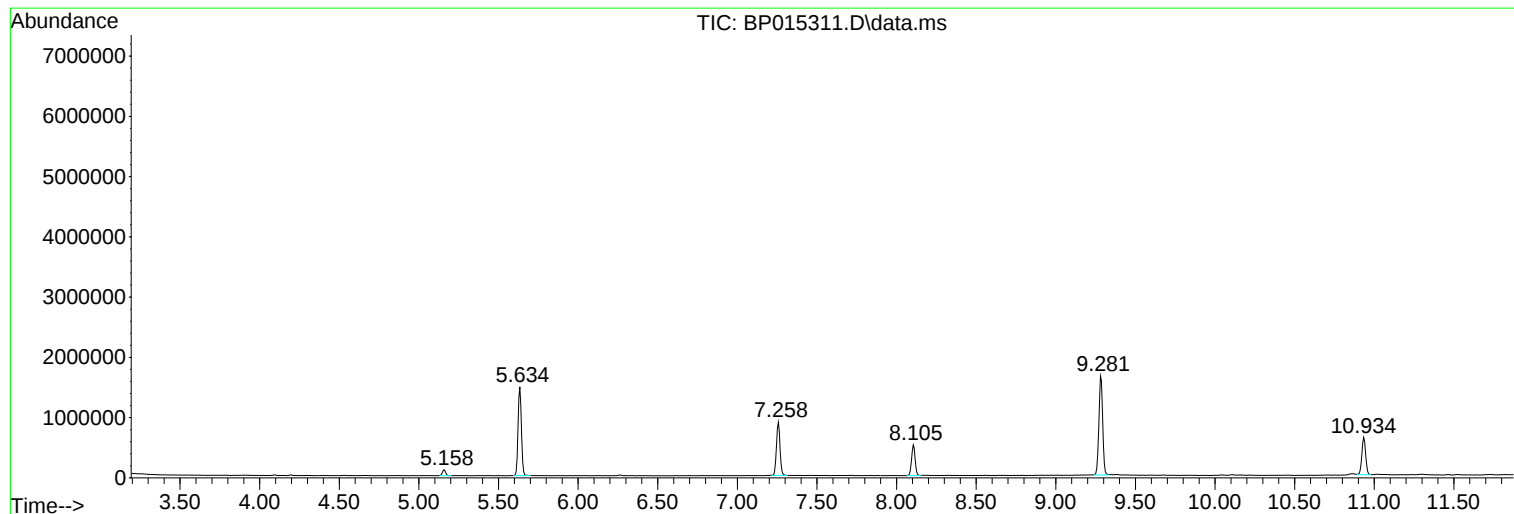
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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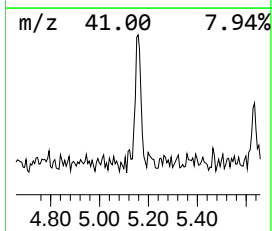
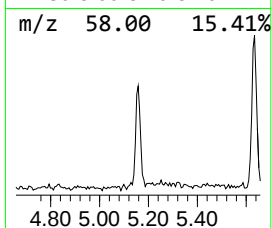
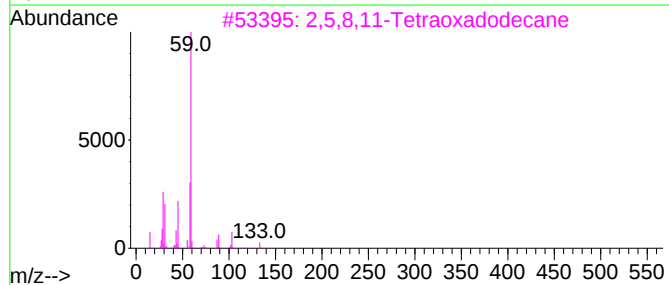
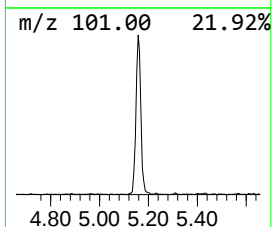
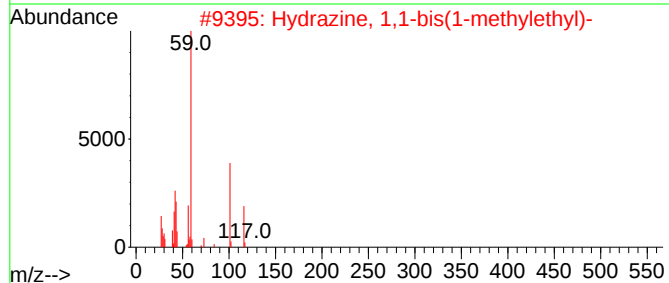
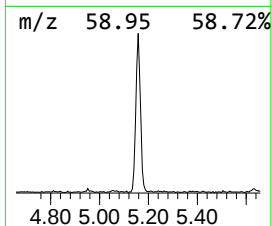
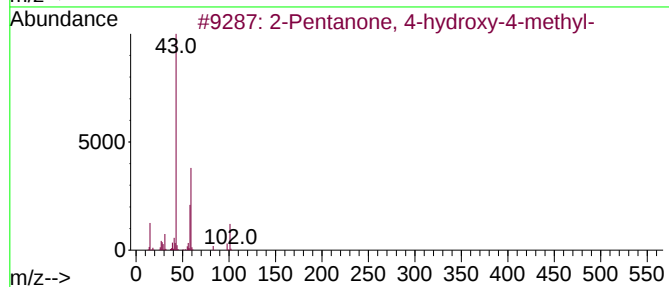
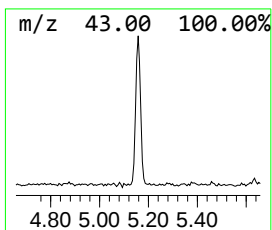
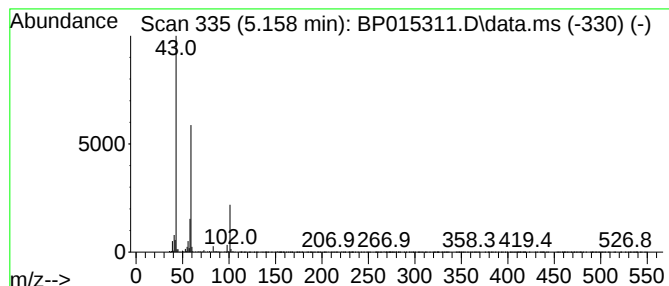
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.158	3.49 ng	138888	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
3			2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Tetraglyme	222	C10H22O5	000143-24-8	23



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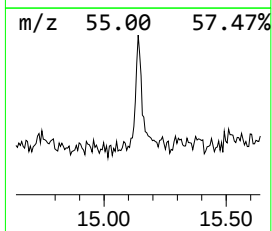
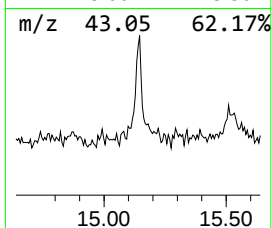
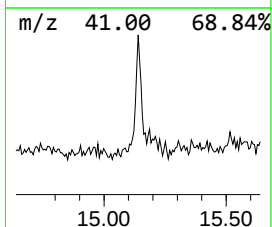
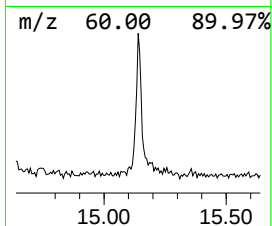
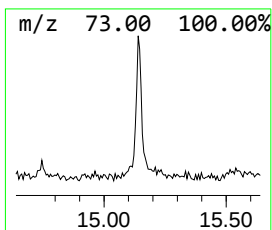
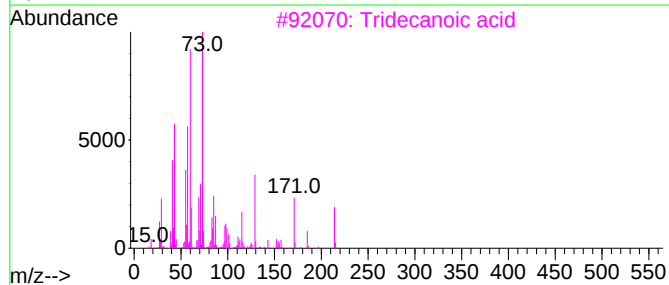
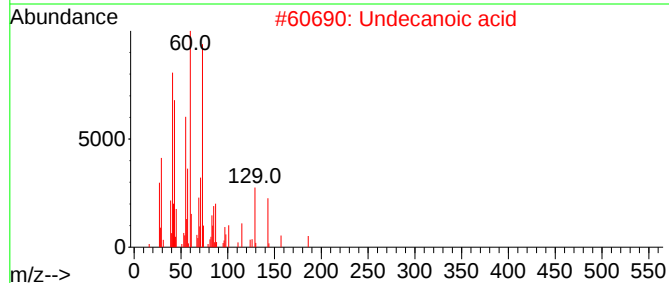
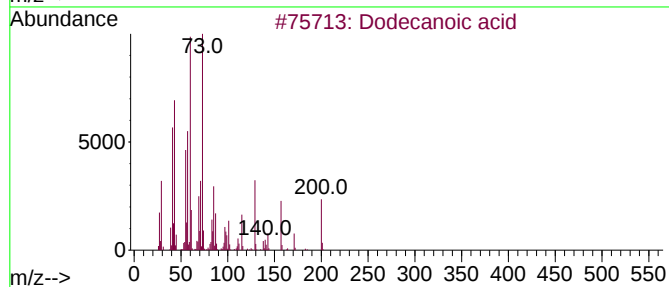
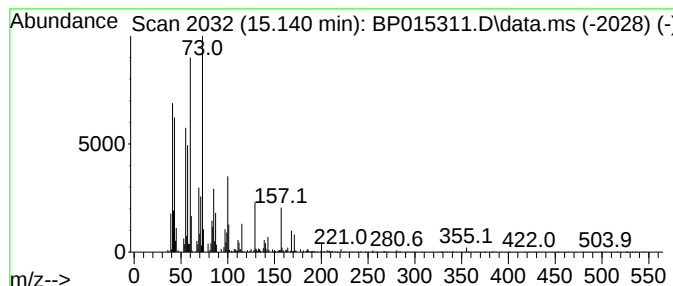
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.140	2.15 ng	138709	Acenaphthene-d10	14.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	81
2			Undecanoic acid	186	C11H22O2	000112-37-8	58
3			Tridecanoic acid	214	C13H26O2	000638-53-9	52
4			Nonanoic acid	158	C9H18O2	000112-05-0	49
5			Octanoic acid	144	C8H16O2	000124-07-2	43



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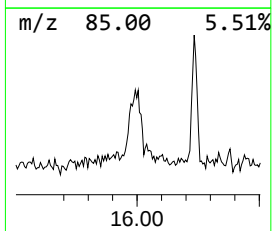
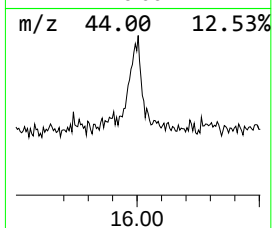
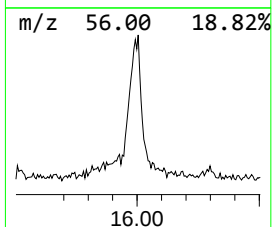
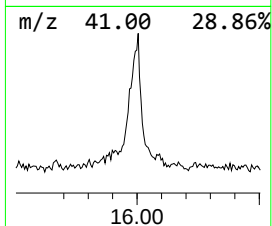
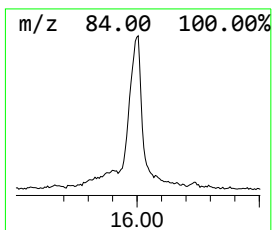
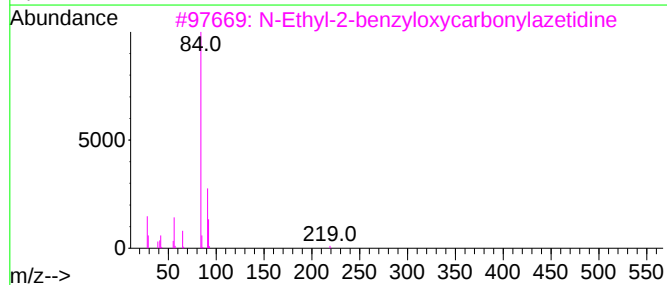
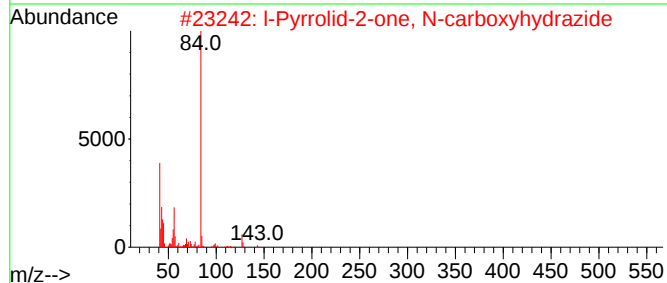
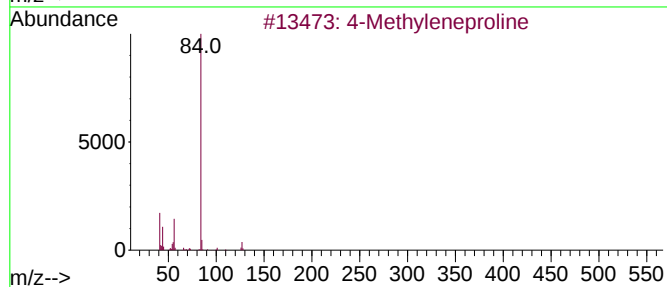
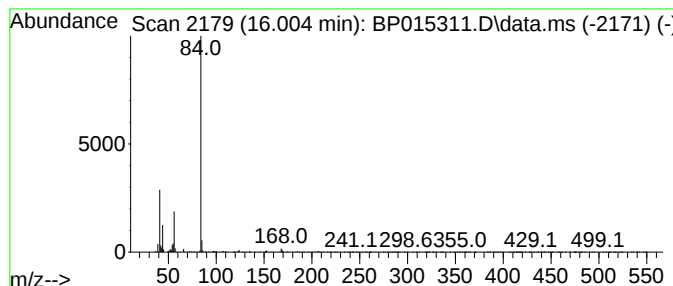
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052423.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Methyleneproline Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	4.76 ng	307658	Acenaphthene-d10	14.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyleneproline	127	C6H9NO2	1000131-14-7	72
2			l-Pyrrolid-2-one, N-carboxyhydra...	143	C5H9N3O2	1000130-58-6	56
3			N-Ethyl-2-benzoyloxycarbonylazeti...	219	C13H17NO2	054773-07-8	50
4			.gamma.-L-glutamyl-L-glutamic acid	276	C10H16N2O7	001116-22-9	50
5			L-Proline, 5-oxo-, methyl ester	143	C6H9NO3	004931-66-2	50



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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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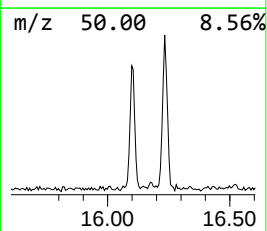
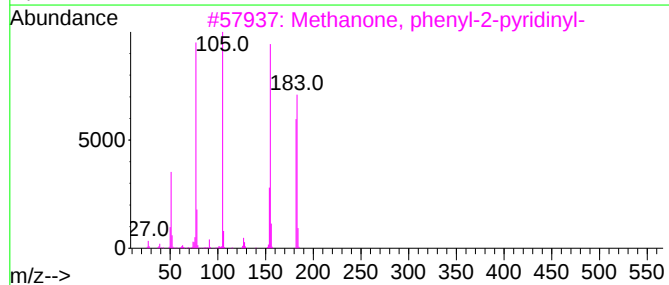
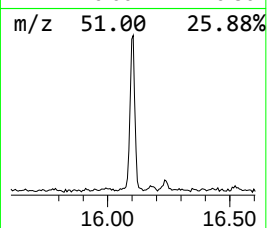
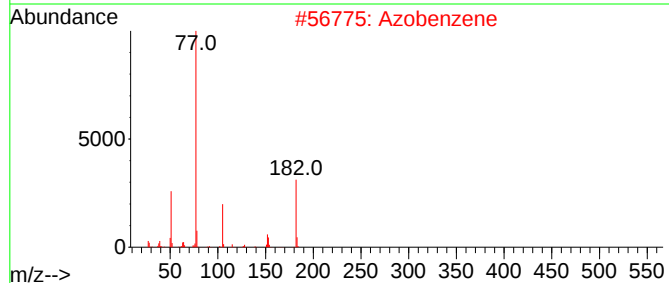
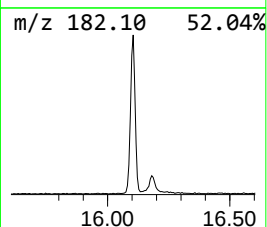
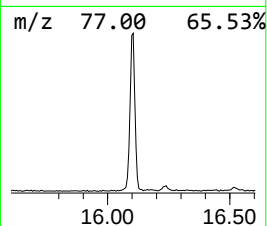
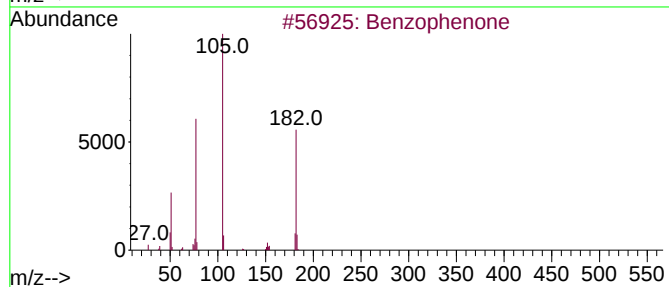
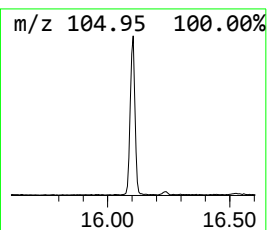
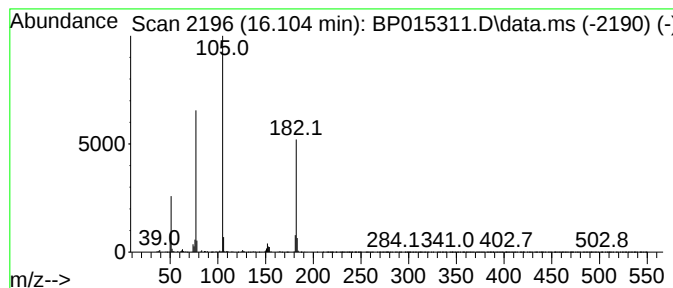
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	7.46 ng	481874	Acenaphthene-d10	14.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
4			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	56
5			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	45



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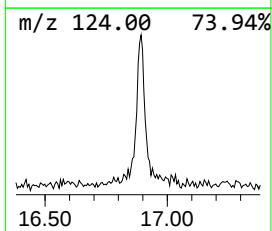
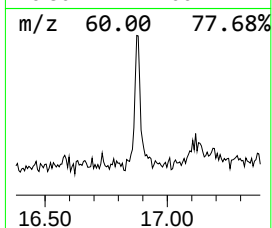
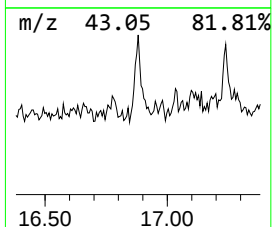
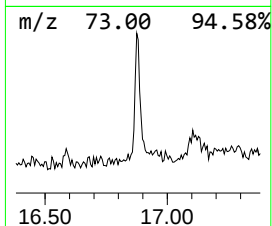
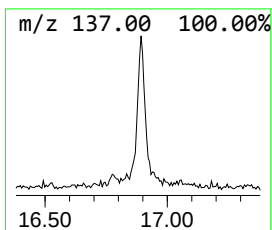
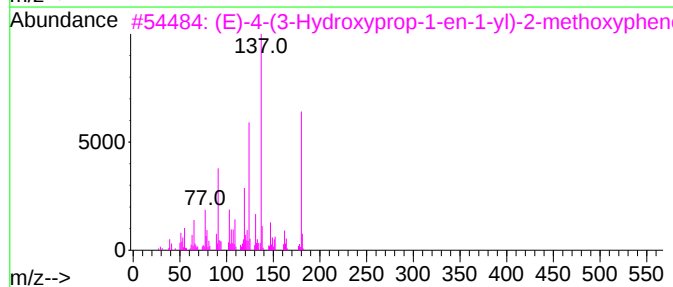
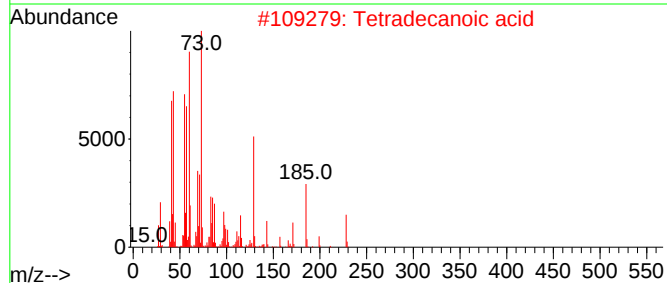
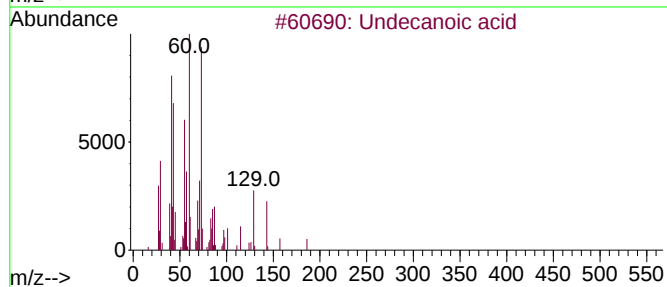
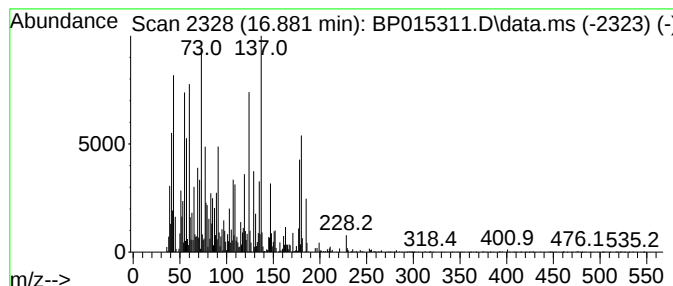
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Peak Number 5 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.881	3.85 ng	307152	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	59
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	56
3			(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	50
4			3-Piperidinamine, 1-(1-methyl-1H...	180	C9H16N4	1251330-45-6	46
5			Benzene, 1-methyl-3-[(2-methylpr...	180	C11H16S	054576-36-2	30



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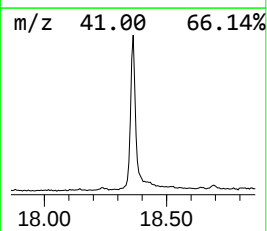
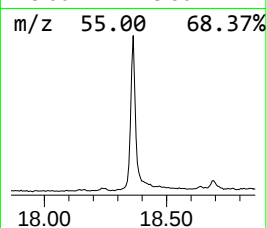
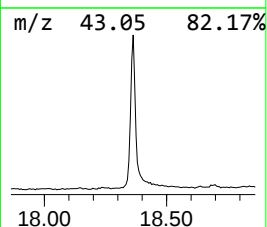
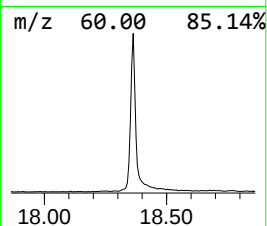
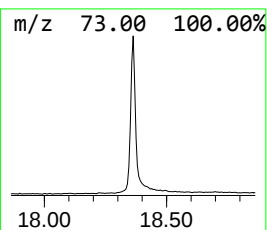
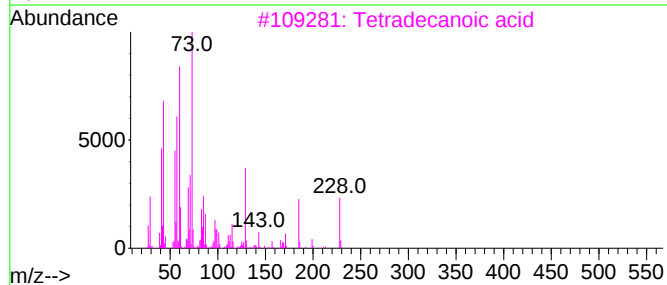
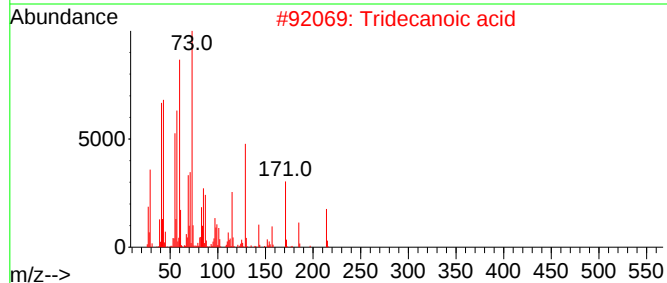
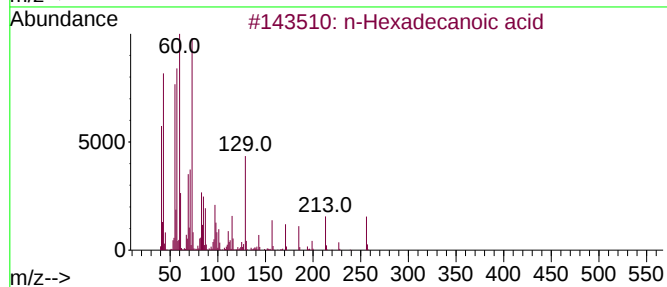
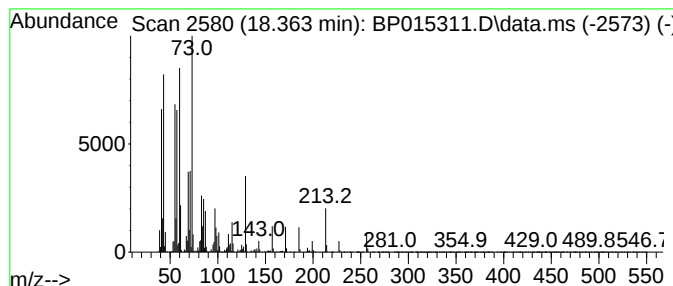
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.363	40.12 ng	3202370	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052623\
Data File : BP015311.D
Acq On : 26 May 2023 16:17
Operator : CG/JU
Sample : 02908-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP02

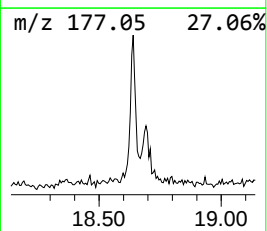
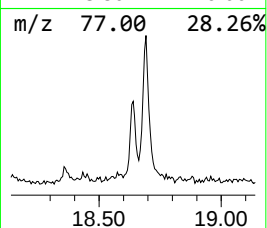
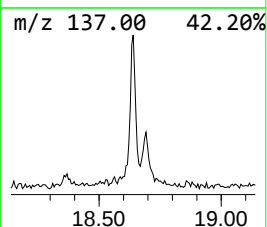
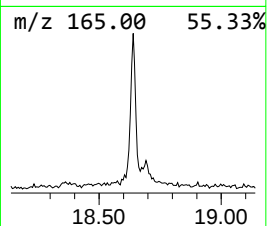
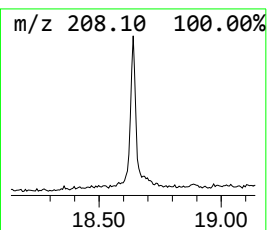
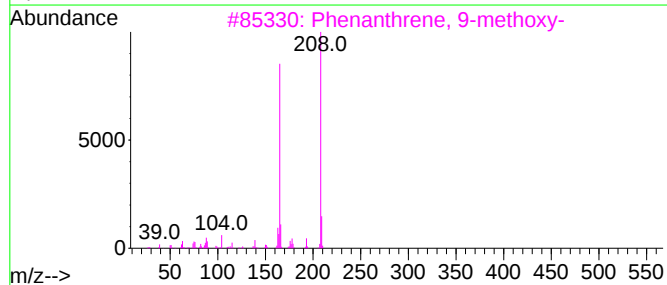
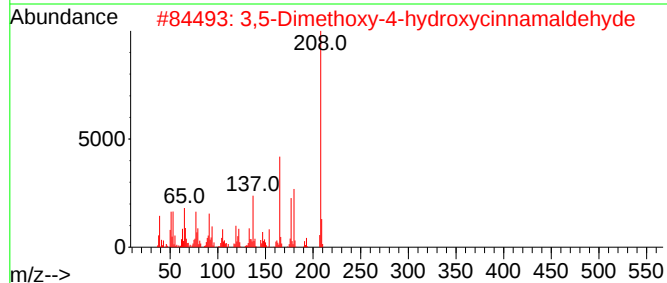
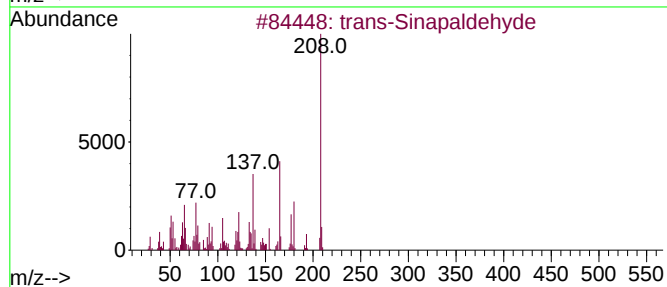
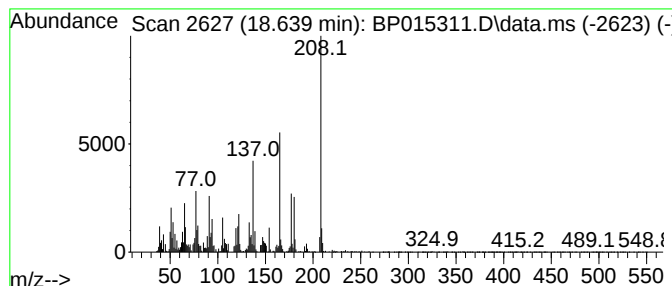
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 trans-Sinapaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.639	4.03 ng	321892	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapaldehyde	208	C11H12O4	004206-58-0	95
2			3,5-Dimethoxy-4-hydroxycinnamaldehyde	208	C11H12O4	087345-53-7	89
3			Phenanthrene, 9-methoxy-	208	C15H12O	005085-74-5	49
4			4-(4-Fluoro-3-methylphenyl)-1,3-bis(4-methoxyphenyl)butane	208	C10H9FN2S	003830-48-6	43
5			1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene	208	C12H16O3	1000313-35-0	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052623\
Data File : BP015311.D
Acq On : 26 May 2023 16:17
Operator : CG/JU
Sample : 02908-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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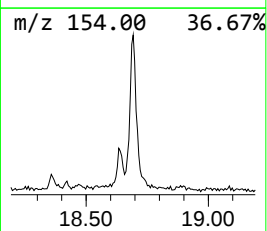
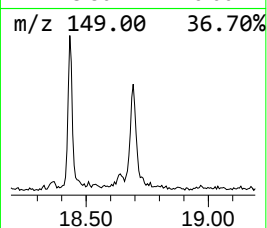
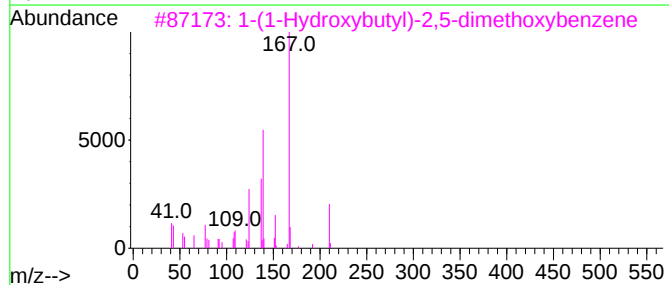
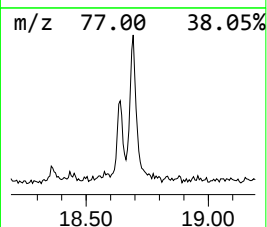
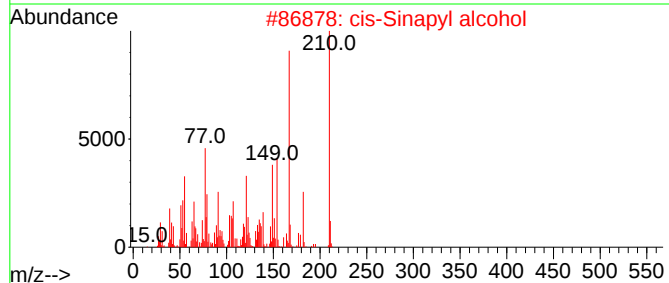
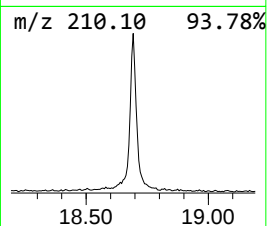
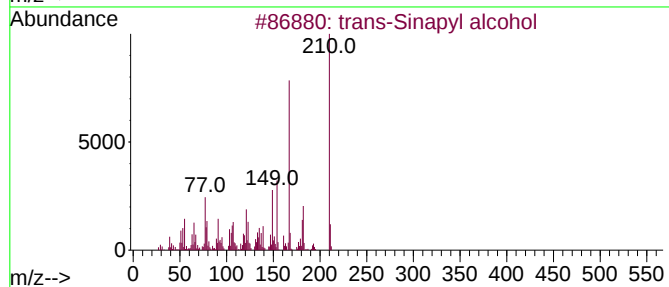
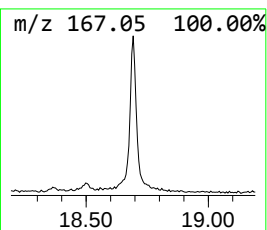
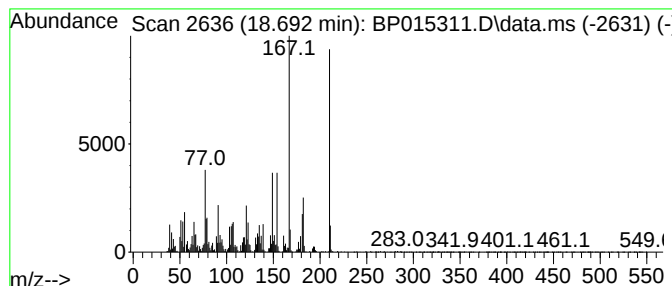
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 trans-Sinapyl alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.692	8.85 ng	706416	Phenanthrene-d10	17.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	96
2		cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	72
3		1-(1-Hydroxybutyl)-2,5-dimethoxy...	210	C12H18O3	149083-03-4	64
4		Syringylacetone	210	C11H14O4	019037-58-2	60
5		4-Ethoxy-2,5-dimethoxybenzaldehyde	210	C11H14O4	1000121-30-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052623\
Data File : BP015311.D
Acq On : 26 May 2023 16:17
Operator : CG/JU
Sample : 02908-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

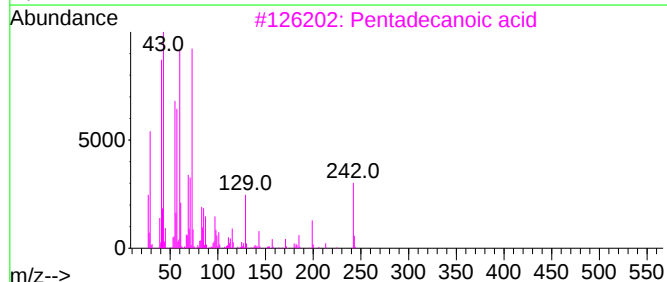
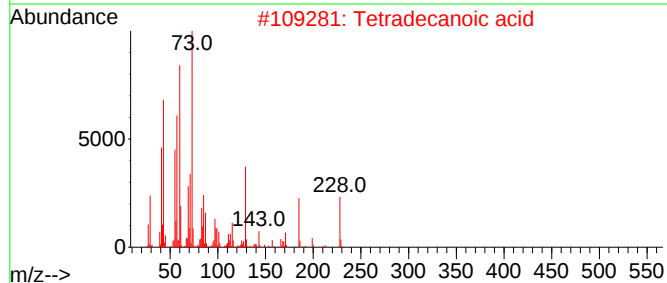
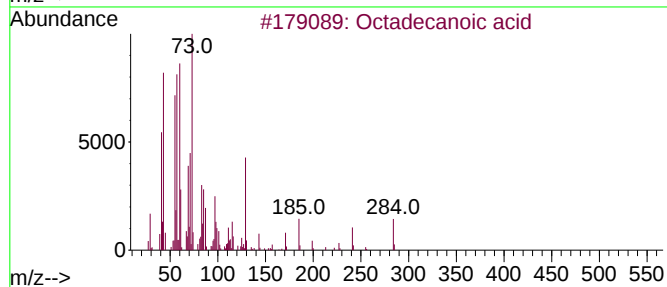
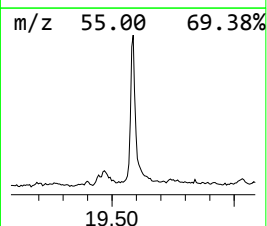
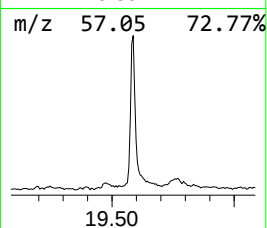
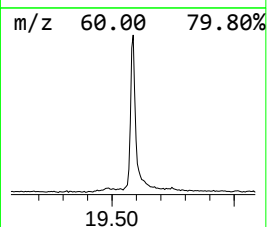
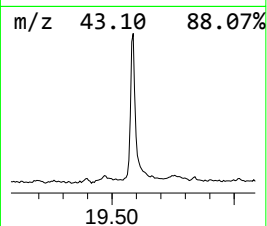
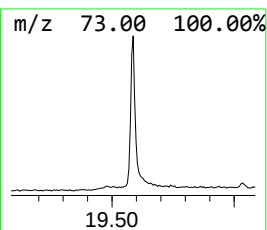
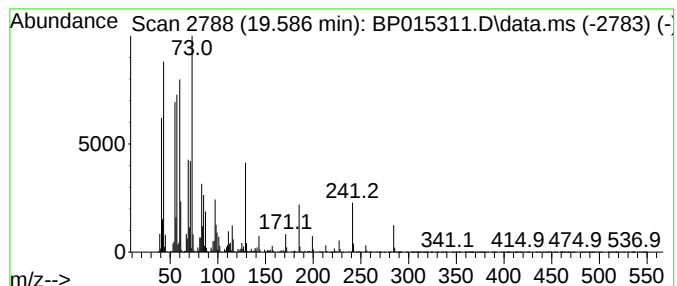
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.586	17.49 ng	1778980	Chrysene-d12	21.580	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052623\
Data File : BP015311.D
Acq On : 26 May 2023 16:17
Operator : CG/JU
Sample : 02908-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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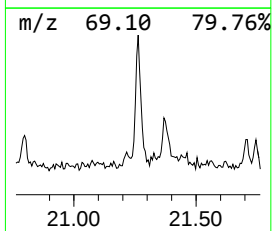
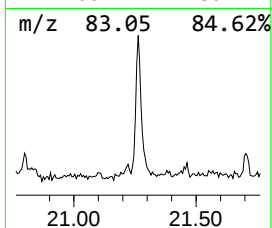
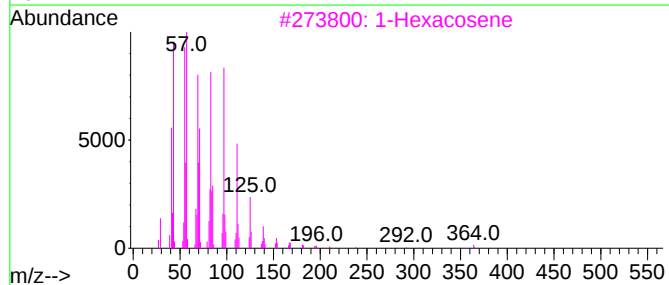
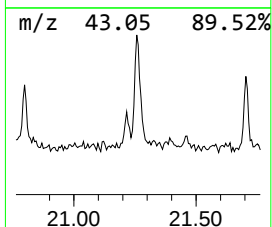
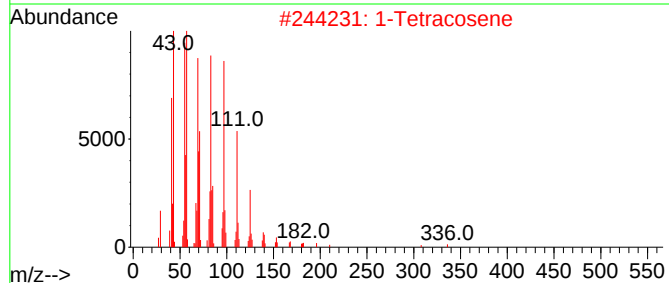
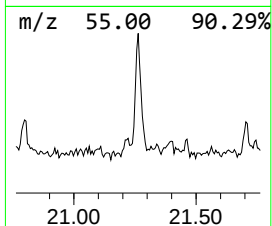
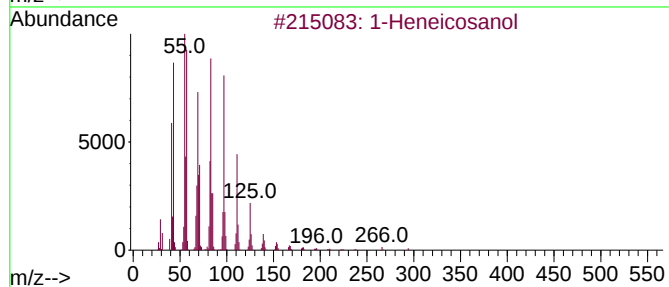
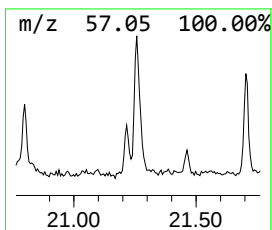
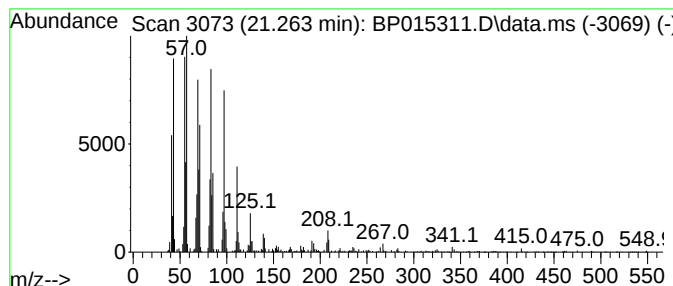
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.263	2.90 ng	294954	Chrysene-d12	21.580

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		1-Tetracosene	336	C24H48	010192-32-2	91
3		1-Hexacosene	364	C26H52	018835-33-1	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052623\
Data File : BP015311.D
Acq On : 26 May 2023 16:17
Operator : CG/JU
Sample : 02908-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TWP02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052423.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-...	5.158	3.5	ng	138888	1	8.105	795438	20.0
Dodecanoic acid	15.140	2.1	ng	138709	3	14.745	1291730	20.0
4-Methyleneproline	16.004	4.8	ng	307658	3	14.745	1291730	20.0
Benzophenone	16.104	7.5	ng	481874	3	14.745	1291730	20.0
Undecanoic acid	16.881	3.9	ng	307152	4	17.498	1596570	20.0
n-Hexadecanoic ...	18.363	40.1	ng	3202370	4	17.498	1596570	20.0
trans-Sinapalde...	18.639	4.0	ng	321892	4	17.498	1596570	20.0
trans-Sinapyl a...	18.692	8.8	ng	706416	4	17.498	1596570	20.0
Octadecanoic acid	19.586	17.5	ng	1778980	5	21.580	2034840	20.0
1-Heneicosanol	21.263	2.9	ng	294954	5	21.580	2034840	20.0