

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061025\
 Data File : BP024892.D
 Acq On : 10 Jun 2025 13:43
 Operator : RC/JU
 Sample : Q2265-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP11-MHL-WC

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-BP060625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024892.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.773	307	312	327	rVB	245899	353633	3.51%	0.638%
2	5.237	385	391	405	rBV	2706522	3963195	39.37%	7.153%
3	6.814	651	659	678	rBV	2377865	4089546	40.62%	7.381%
4	7.608	786	794	802	rBV	763702	1202409	11.94%	2.170%
5	8.761	982	990	1006	rBV	1476928	2649935	26.32%	4.783%
6	10.372	1257	1264	1277	rBV	945692	1647518	16.36%	2.974%
7	12.849	1678	1685	1707	rBV	4138776	6426233	63.83%	11.599%
8	14.248	1916	1923	1939	rBV	1462013	2258844	22.44%	4.077%
9	15.095	2057	2067	2077	rBV	148502	275277	2.73%	0.497%
10	15.643	2153	2160	2175	rBV	804042	1198912	11.91%	2.164%
11	15.778	2175	2183	2201	rBV	3101542	5415418	53.79%	9.774%
12	16.219	2247	2258	2263	rBV	127911	203622	2.02%	0.368%
13	17.060	2395	2401	2412	rBV2	1717977	2676091	26.58%	4.830%
14	17.748	2509	2518	2535	rBV	491505	853722	8.48%	1.541%
15	18.007	2556	2562	2569	rBV	943053	1380728	13.71%	2.492%
16	18.066	2569	2572	2585	rVB	143884	283550	2.82%	0.512%
17	18.442	2631	2636	2642	rBV3	176814	261619	2.60%	0.472%
18	19.207	2760	2766	2778	rBV10	50132	178147	1.77%	0.322%
19	19.331	2782	2787	2804	rBV2	323001	658921	6.55%	1.189%
20	19.783	2859	2864	2874	rBV	7962067	10067505	100.00%	18.171%
21	20.642	3007	3010	3014	rBV	139820	161741	1.61%	0.292%
22	21.154	3093	3097	3106	rBV	397567	677171	6.73%	1.222%
23	21.483	3148	3153	3165	rBV2	1931395	3182631	31.61%	5.744%
24	21.719	3190	3193	3199	rVB	180447	235014	2.33%	0.424%
25	22.342	3295	3299	3306	rVB2	186747	316727	3.15%	0.572%
26	23.019	3410	3414	3418	rBV	288883	520877	5.17%	0.940%
27	23.236	3446	3451	3458	rVB	418571	701568	6.97%	1.266%
28	24.736	3697	3706	3717	rVB	1459825	3564039	35.40%	6.433%

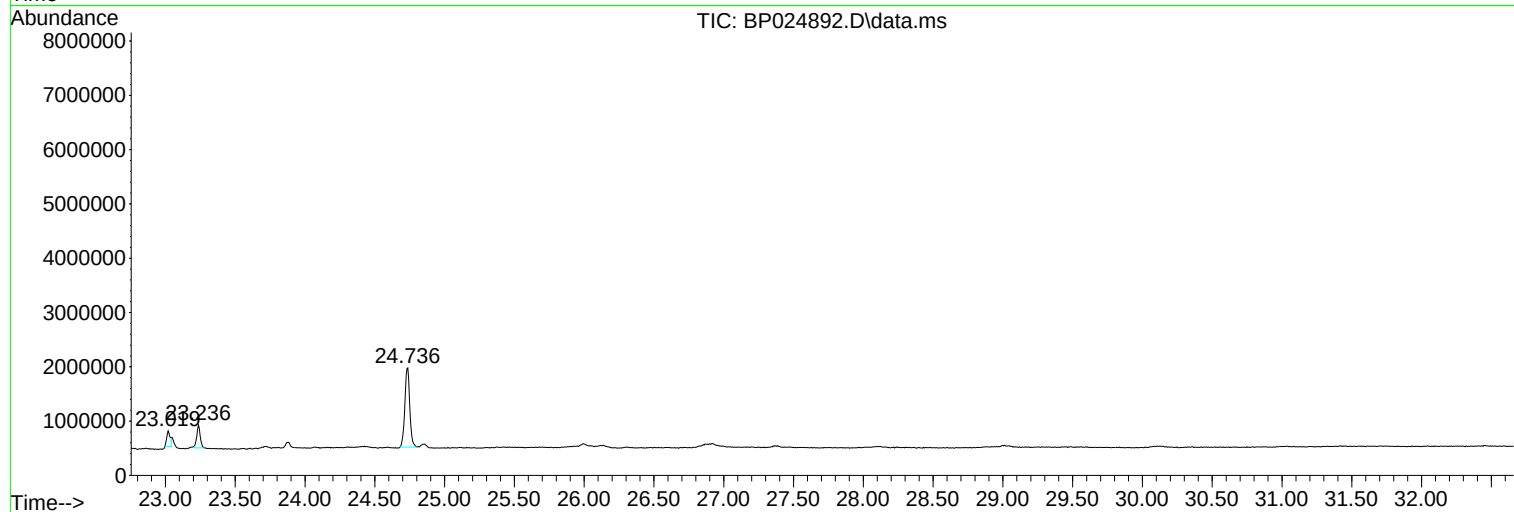
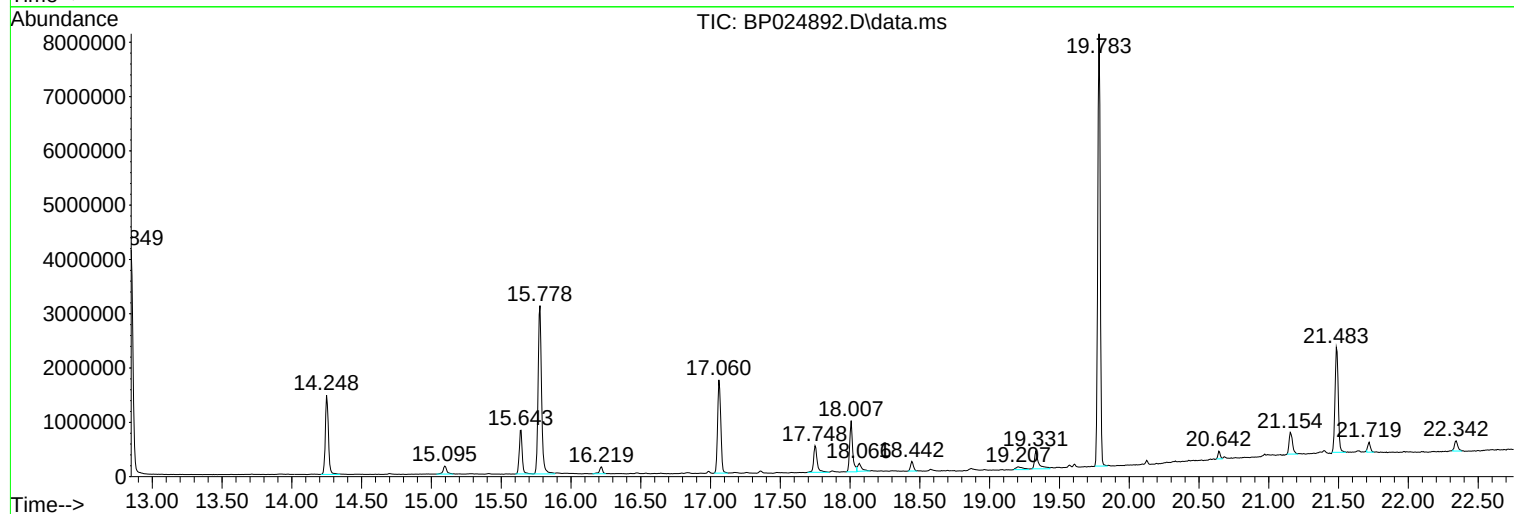
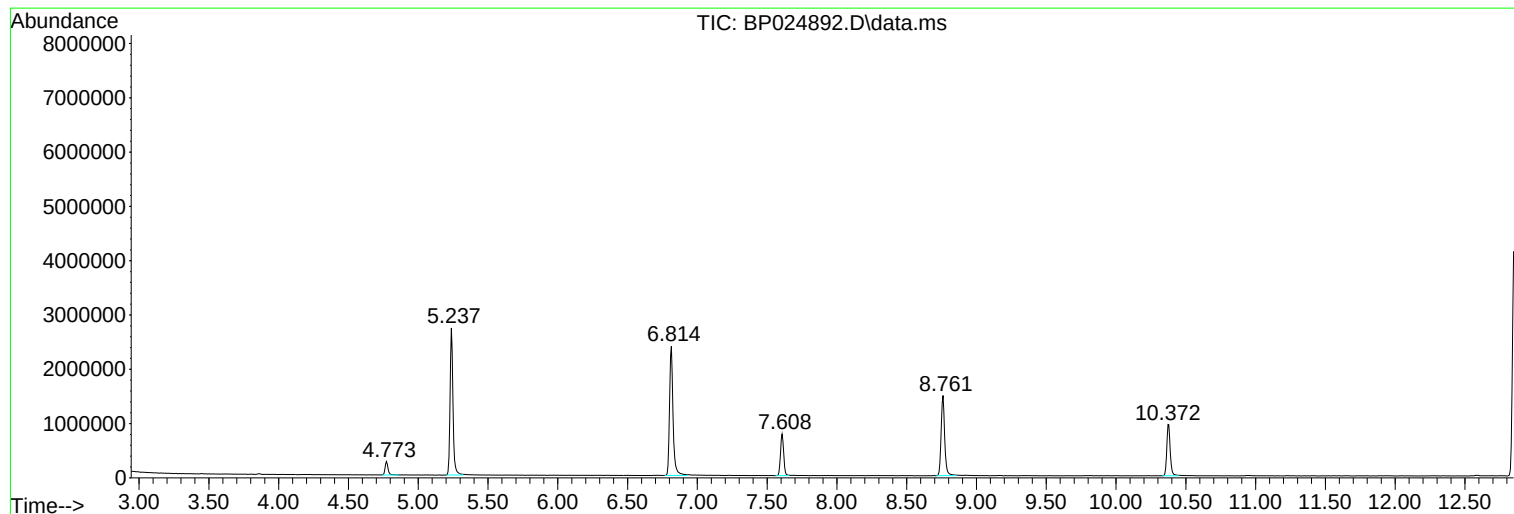
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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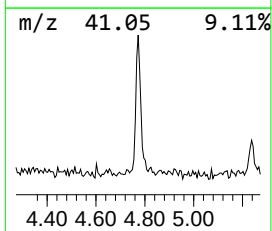
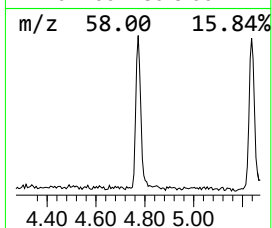
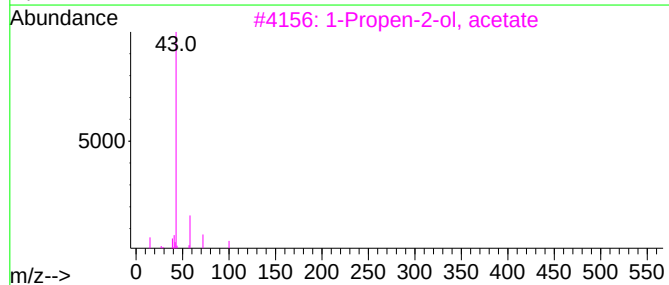
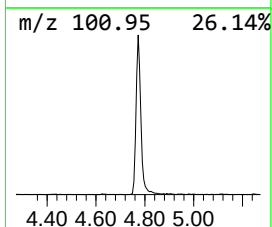
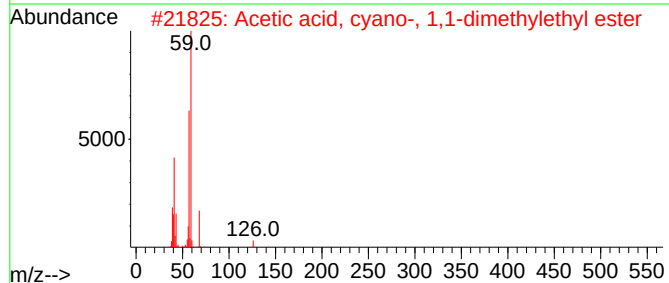
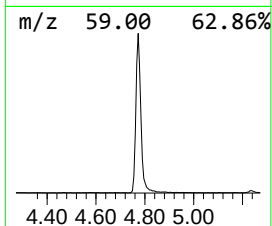
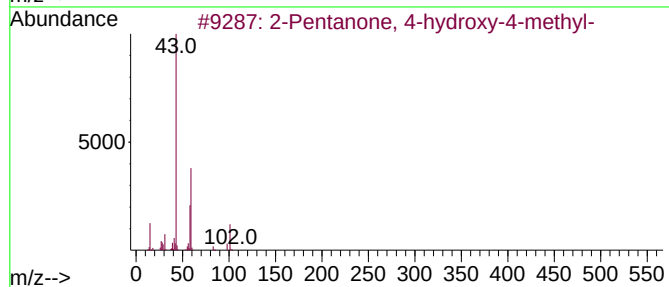
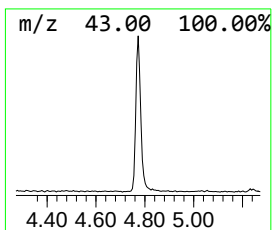
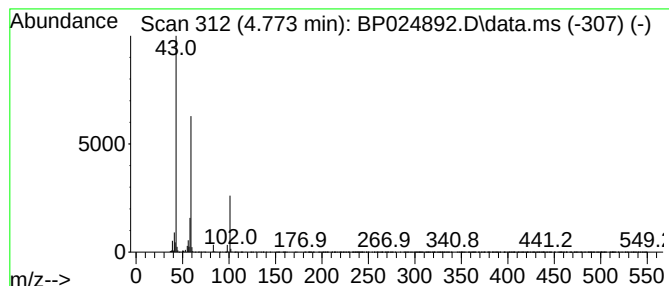
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.773	5.88 ng	353633	1,4-Dichlorobenzene-d4	7.608

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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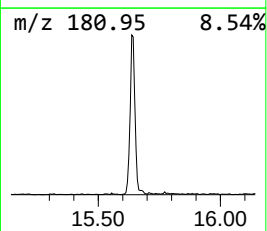
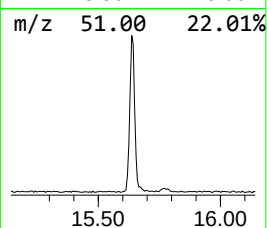
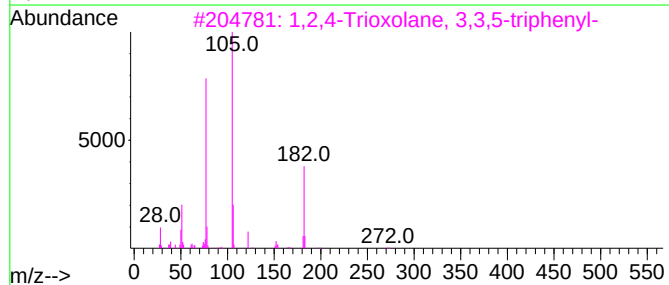
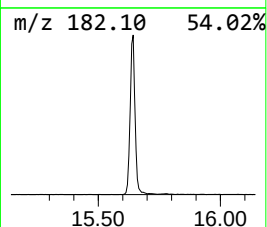
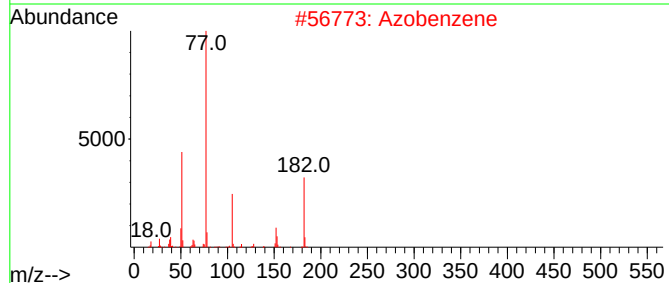
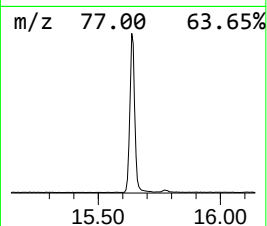
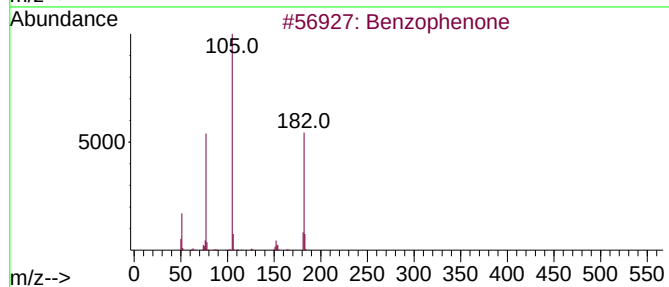
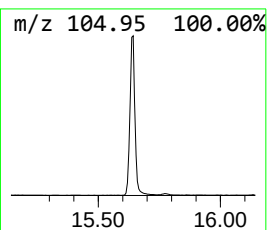
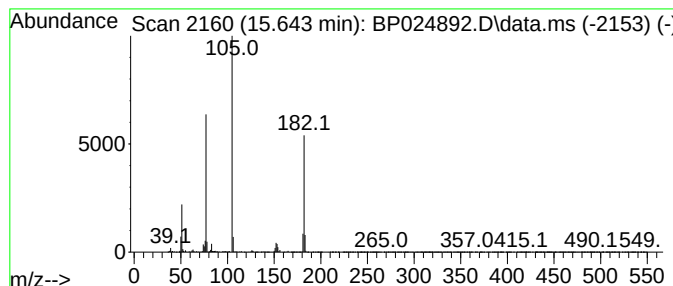
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.643	10.62 ng	1198910	Acenaphthene-d10	14.249

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			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50
4			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
5			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	42



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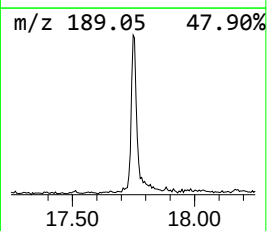
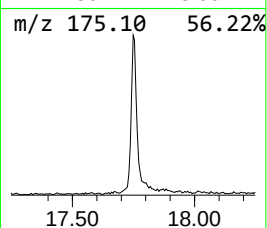
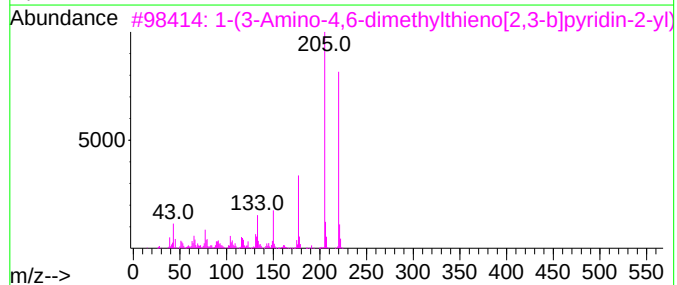
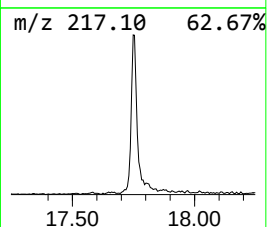
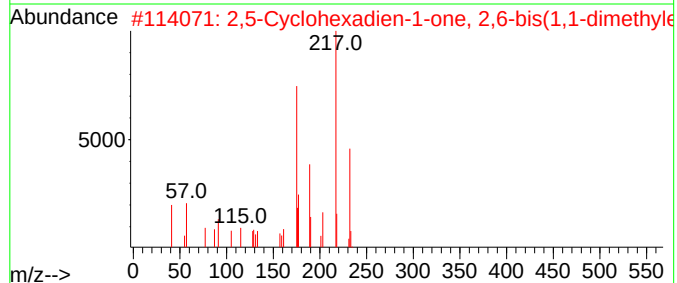
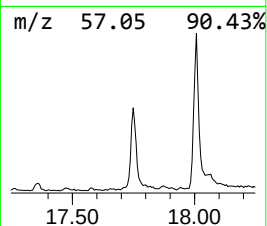
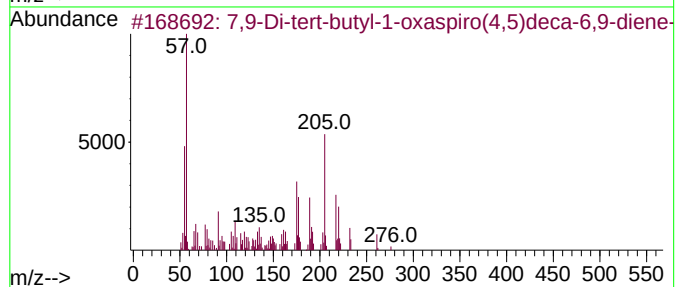
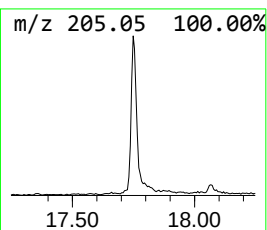
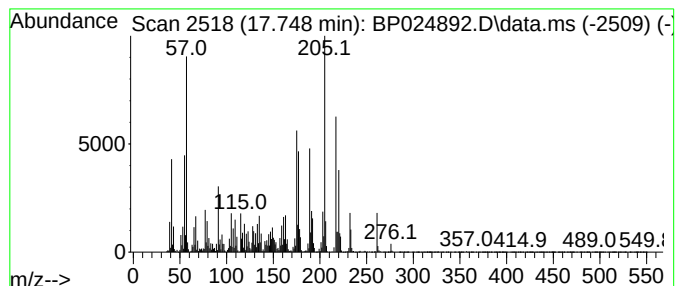
Instrument :
BNA_P
ClientSampleId :
TP11-MHL-WC

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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 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.748	6.38 ng	853722	Phenanthrene-d10		17.060	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...		276	C17H24O3	082304-66-3	99
2	2,5-Cyclohexadien-1-one, 2,6-bis...		232	C16H24O	006738-27-8	86
3	1-(3-Amino-4,6-dimethylthieno[2,...		220	C11H12N2OS	052505-42-7	50
4	2,5-di-tert-Butyl-1,4-benzoquinone		220	C14H20O2	002460-77-7	50
5	Butylated Hydroxytoluene		220	C15H24O	000128-37-0	49



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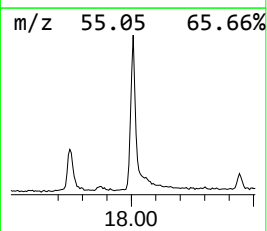
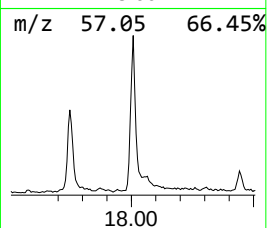
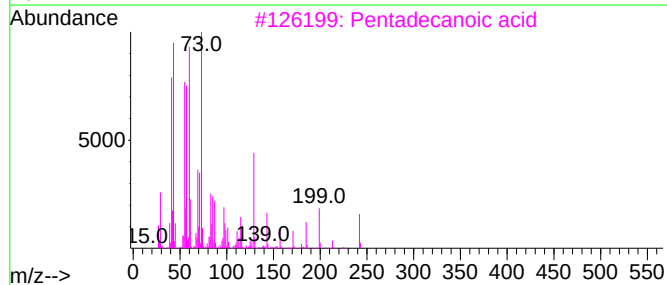
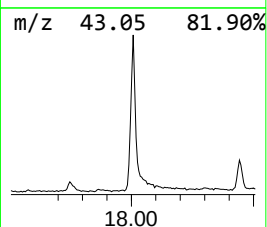
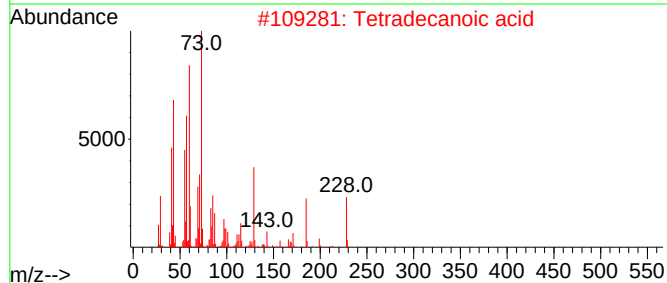
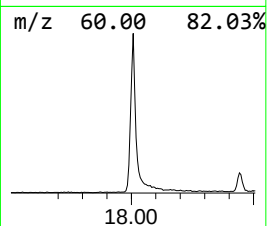
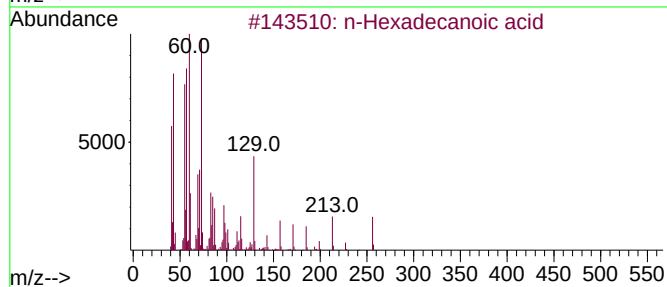
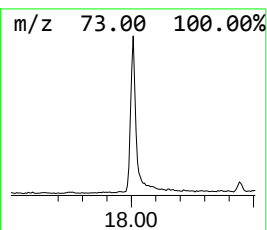
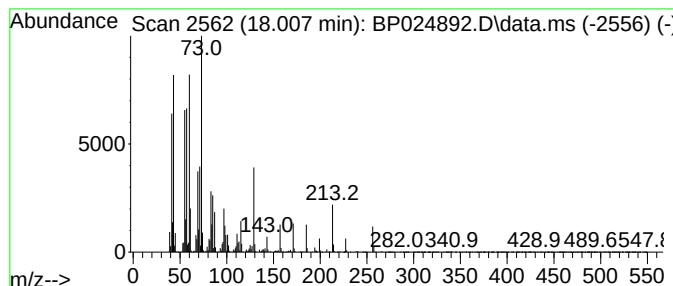
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.007	10.32 ng	1380730	Phenanthrene-d10	17.060

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			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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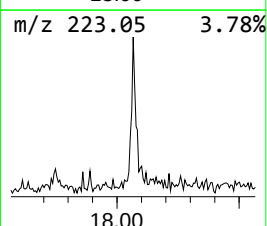
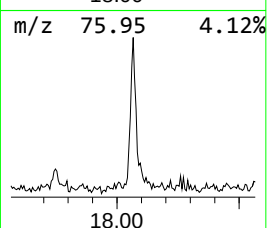
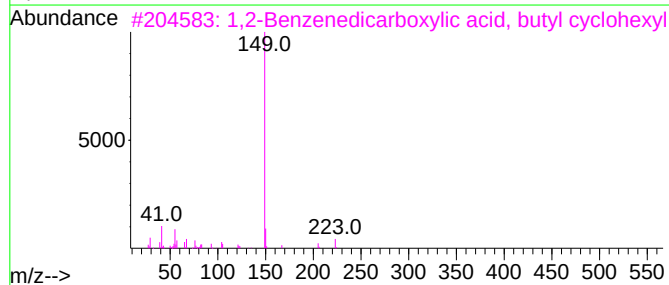
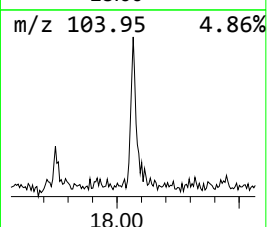
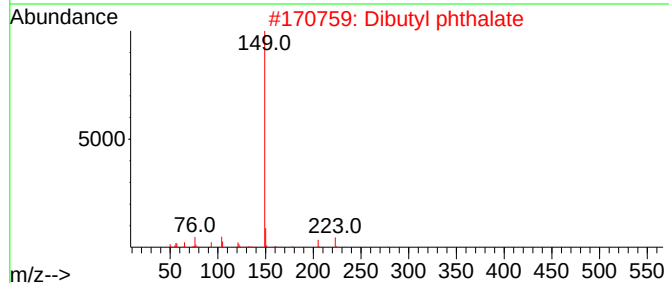
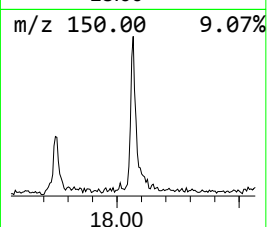
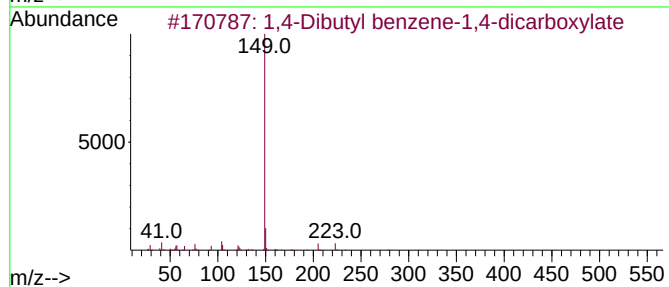
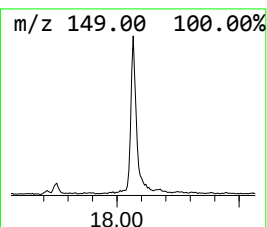
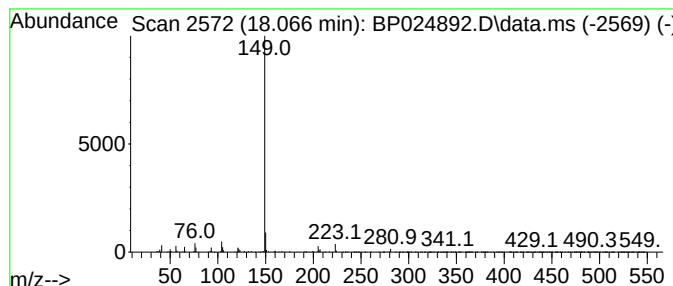
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1,4-Dibutyl benzene-1,4-dic... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.066	2.12 ng	283550	Phenanthrene-d10	17.060

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dibutyl benzene-1,4-dicarbox...	278	C16H22O4	001962-75-0	95
2			Dibutyl phthalate	278	C16H22O4	000084-74-2	93
3			1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	86
4			1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	86
5			Diamyl phthalate	306	C18H26O4	000131-18-0	72



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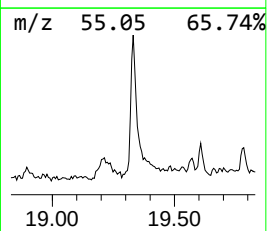
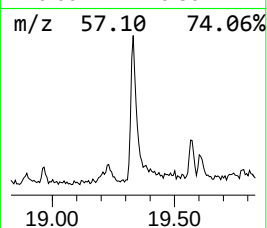
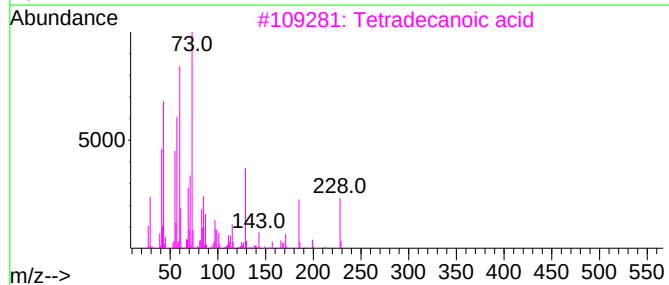
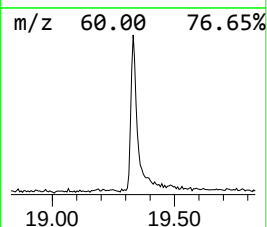
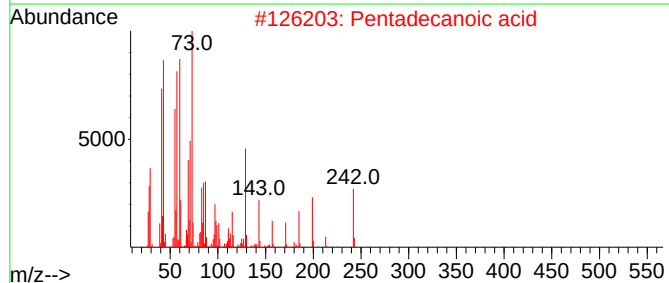
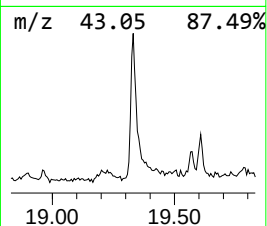
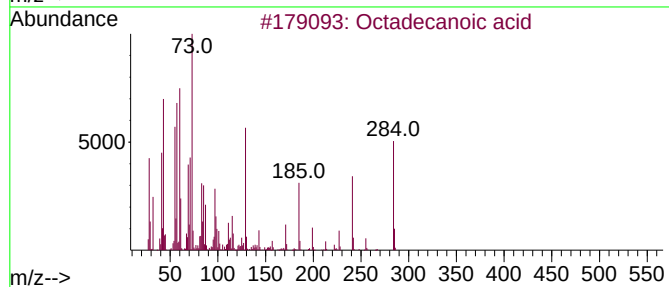
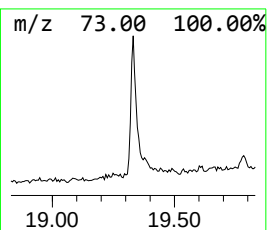
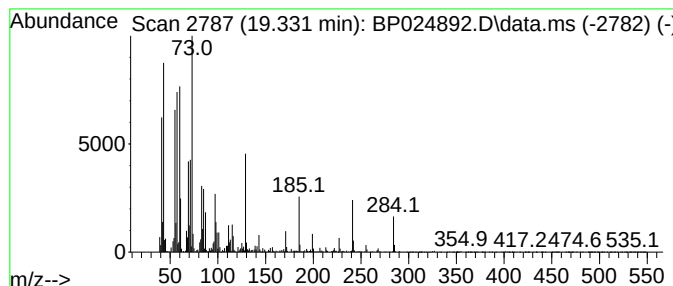
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
19.331	4.14 ng	658921	Chrysene-d12	21.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061025\
Data File : BP024892.D
Acq On : 10 Jun 2025 13:43
Operator : RC/JU
Sample : Q2265-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP11-MHL-WC

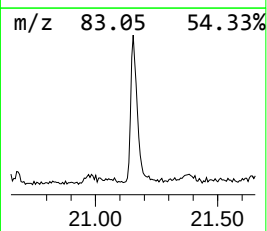
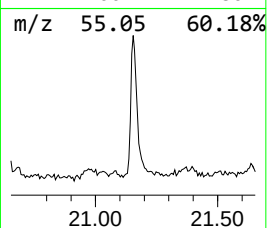
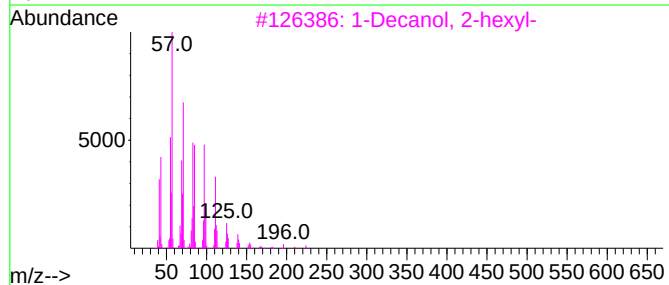
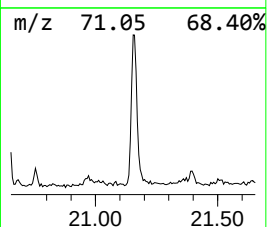
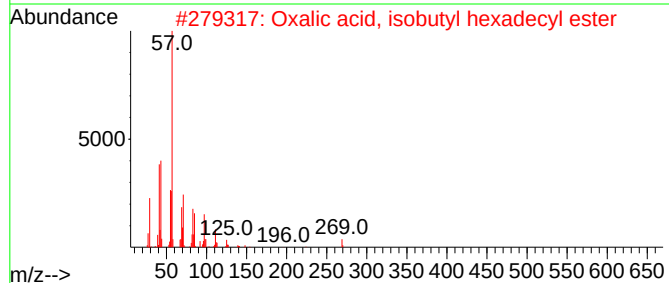
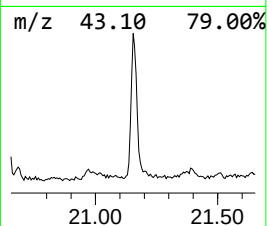
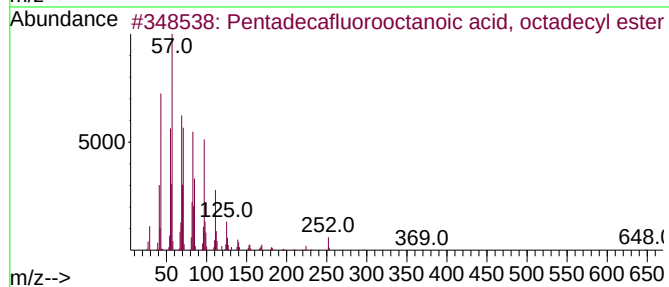
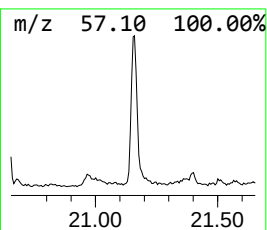
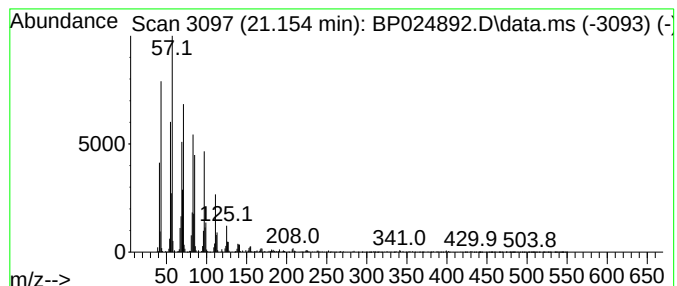
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.154	4.26 ng	677171	Chrysene-d12	21.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061025\
Data File : BP024892.D
Acq On : 10 Jun 2025 13:43
Operator : RC/JU
Sample : Q2265-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP11-MHL-WC

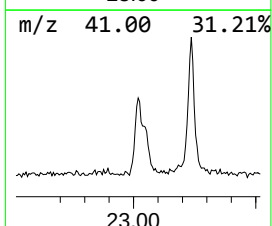
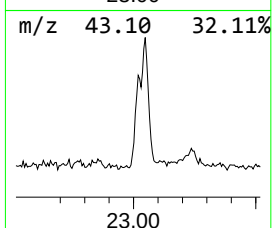
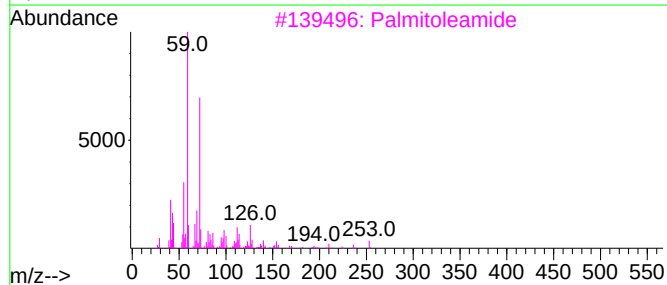
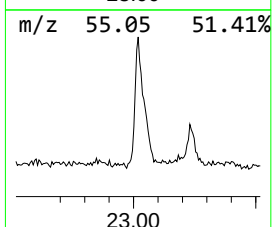
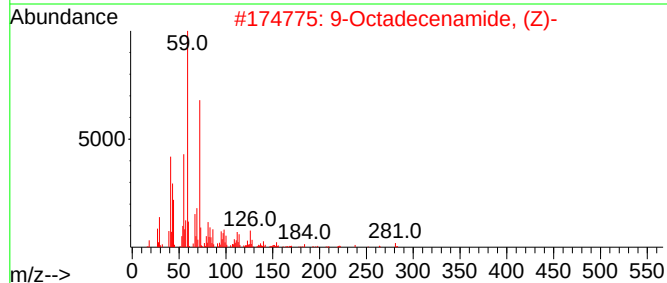
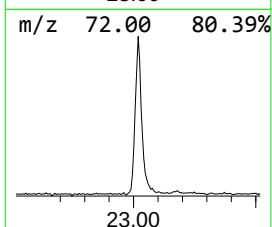
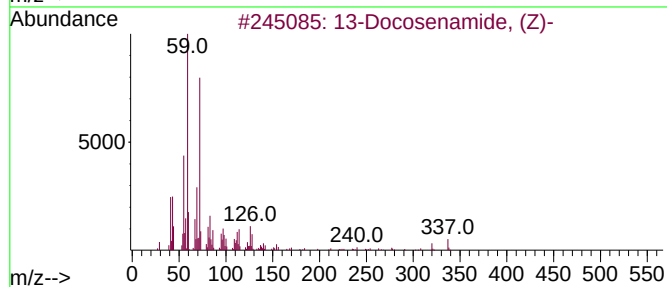
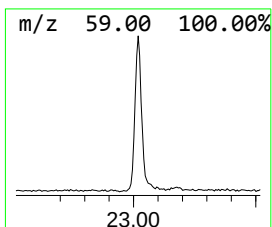
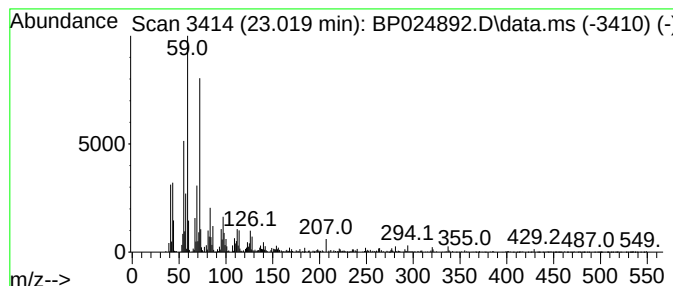
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.019	3.27 ng	520877	Chrysene-d12	21.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	99
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
3			Palmitoleamide	253	C16H31NO	106010-22-4	86
4			9-Octadecenamide	281	C18H35NO	003322-62-1	53
5			Propionamide, 3-bromo-N-propyl-N...	249	C10H20BrNO	1000438-64-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061025\
Data File : BP024892.D
Acq On : 10 Jun 2025 13:43
Operator : RC/JU
Sample : Q2265-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP11-MHL-WC

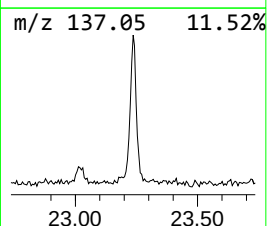
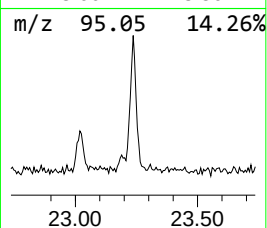
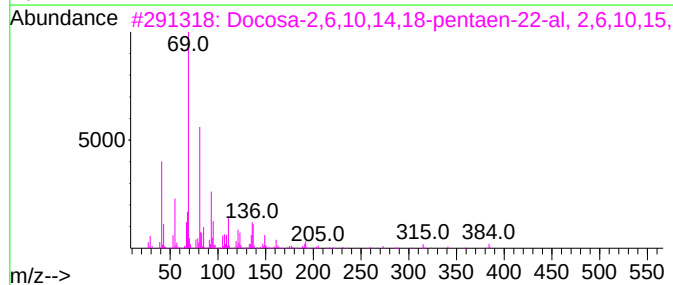
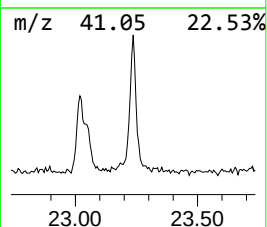
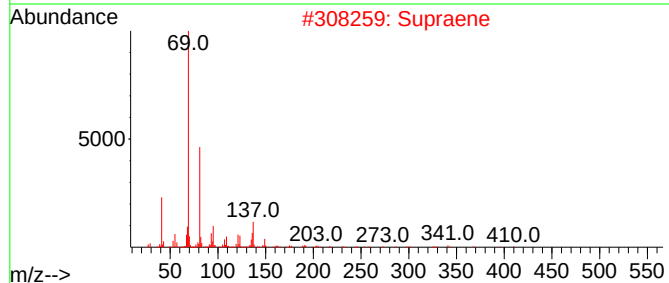
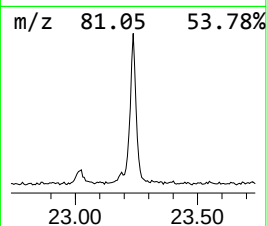
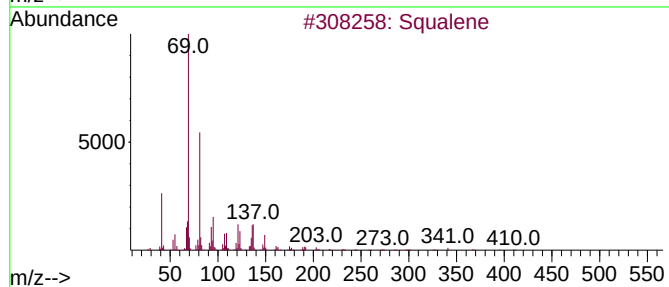
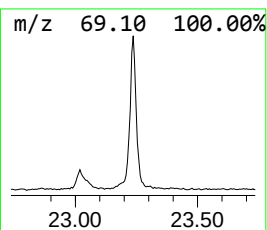
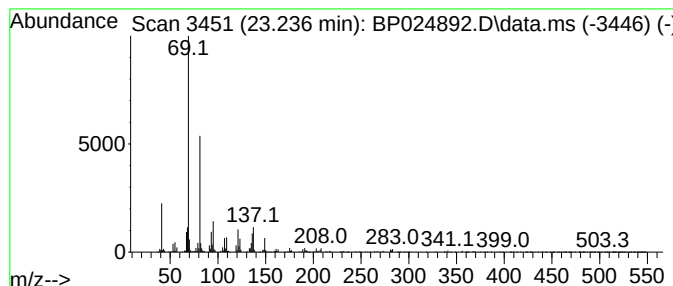
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.236	3.94 ng	701568	Perylene-d12	24.730

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	98
2			Supraene	410	C30H50	007683-64-9	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
5			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061025\
Data File : BP024892.D
Acq On : 10 Jun 2025 13:43
Operator : RC/JU
Sample : Q2265-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP11-MHL-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060625.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-...	4.773	5.9	ng	353633	1	7.608	1202410	20.0
Benzophenone	15.643	10.6	ng	1198910	3	14.249	2258840	20.0
7,9-Di-tert-but...	17.748	6.4	ng	853722	4	17.060	2676090	20.0
n-Hexadecanoic ...	18.007	10.3	ng	1380730	4	17.060	2676090	20.0
1,4-Dibutyl ben...	18.066	2.1	ng	283550	4	17.060	2676090	20.0
Octadecanoic acid	19.331	4.1	ng	658921	5	21.483	3182630	20.0
Pentadecafluoro...	21.154	4.3	ng	677171	5	21.483	3182630	20.0
13-Docosenamide...	23.019	3.3	ng	520877	5	21.483	3182630	20.0
Squalene	23.236	3.9	ng	701568	6	24.730	3564040	20.0