

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
 Data File : BP025380.D
 Acq On : 13 Aug 2025 11:59
 Operator : CG/JU
 Sample : Q2820-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 82H-W

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-BP080525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.967	3	5	13	rVB3	125453	205010	3.51%	0.510%
2	3.043	13	18	32	rVB	758013	1107095	18.96%	2.756%
3	4.949	337	342	350	rVB	173099	254842	4.37%	0.634%
4	5.413	413	421	428	rBV	1841120	2765613	47.37%	6.885%
5	6.972	677	686	696	rBV	1757666	2810051	48.13%	6.996%
6	7.802	818	827	834	rBV	614319	996010	17.06%	2.480%
7	8.937	1013	1020	1032	rVB	1137129	1888165	32.34%	4.701%
8	10.572	1291	1298	1306	rBV	783672	1369004	23.45%	3.408%
9	13.031	1709	1716	1728	rBV	2710753	4009379	68.68%	9.982%
10	14.419	1943	1952	1959	rBV	1194047	1789275	30.65%	4.455%
11	15.442	2121	2126	2130	rBV	95055	137699	2.36%	0.343%
12	15.607	2148	2154	2158	rBV3	40226	71409	1.22%	0.178%
13	15.801	2182	2187	2194	rVB	313246	429714	7.36%	1.070%
14	15.925	2203	2208	2218	rVB	2317530	3218557	55.13%	8.013%
15	16.031	2222	2226	2234	rBV5	45306	74582	1.28%	0.186%
16	16.195	2251	2254	2258	rVB	48502	59471	1.02%	0.148%
17	16.289	2265	2270	2275	rBV	115454	184328	3.16%	0.459%
18	16.354	2276	2281	2288	rBV3	119281	306996	5.26%	0.764%
19	16.419	2288	2292	2296	rVB2	130519	174302	2.99%	0.434%
20	16.460	2296	2299	2303	rBV	107448	141383	2.42%	0.352%
21	16.507	2303	2307	2310	rBV3	48313	82439	1.41%	0.205%
22	16.619	2322	2326	2333	rVB3	147963	281324	4.82%	0.700%
23	16.689	2333	2338	2342	rBV	111747	159965	2.74%	0.398%
24	16.766	2347	2351	2357	rVB2	73946	117501	2.01%	0.293%
25	17.225	2423	2429	2435	rBV2	1330474	2032751	34.82%	5.061%
26	18.177	2585	2591	2599	rBV	1550027	2349224	40.24%	5.849%
27	18.442	2632	2636	2639	rBV	154546	211280	3.62%	0.526%
28	18.489	2639	2644	2652	rVB	253196	427296	7.32%	1.064%
29	19.195	2761	2764	2772	rVB	130537	164948	2.83%	0.411%
30	19.501	2812	2816	2826	rBV	475924	688628	11.80%	1.714%
31	19.730	2852	2855	2858	rBV	60167	82034	1.41%	0.204%
32	19.954	2888	2893	2901	rBV	4557011	5837900	100.00%	14.534%
33	21.354	3127	3131	3142	rVB2	401834	683075	11.70%	1.701%
34	21.677	3180	3186	3193	rBV2	1526997	2428323	41.60%	6.046%
35	25.071	3755	3763	3776	rVB	1007479	2627328	45.00%	6.541%

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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-BP080525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

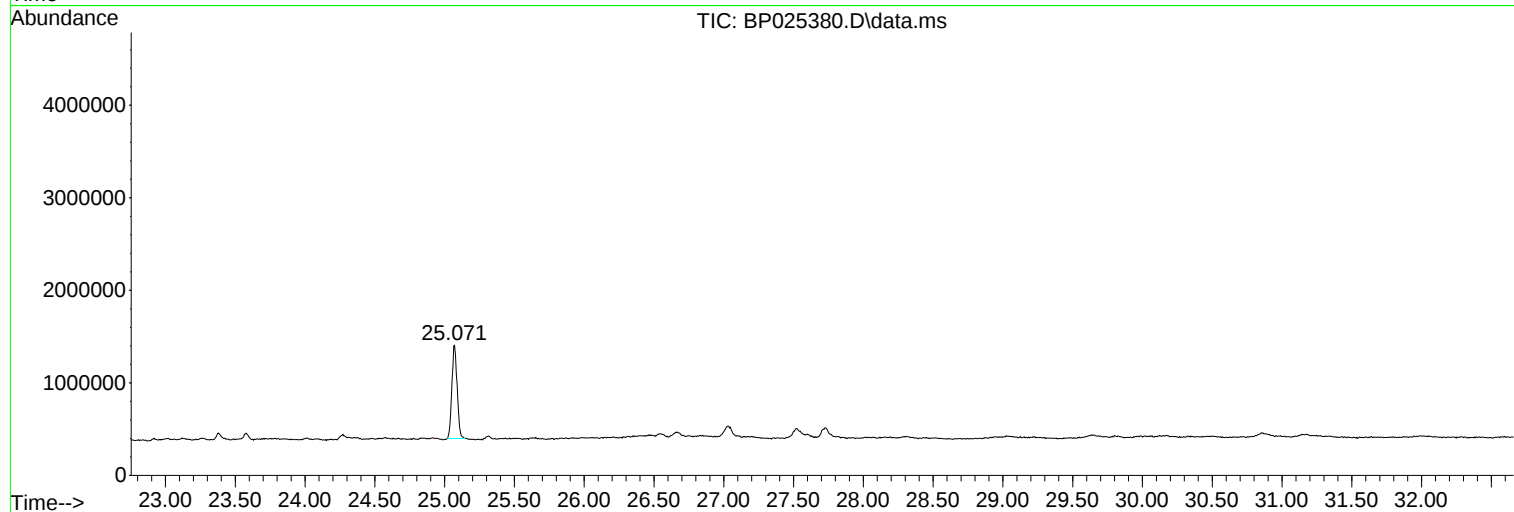
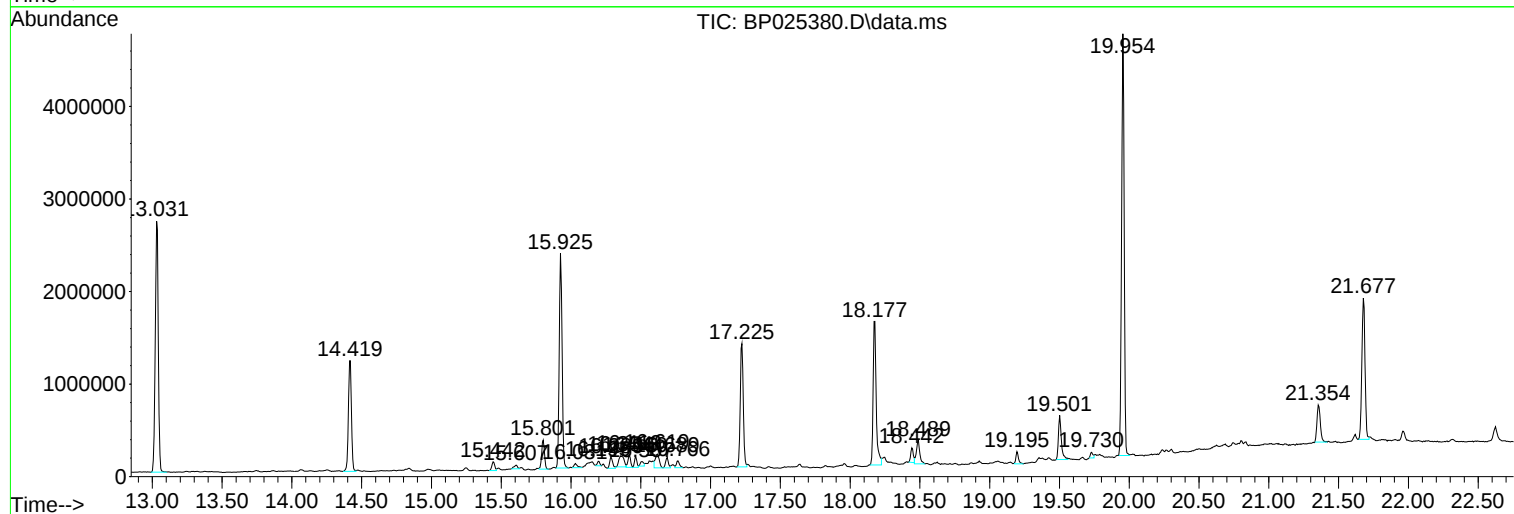
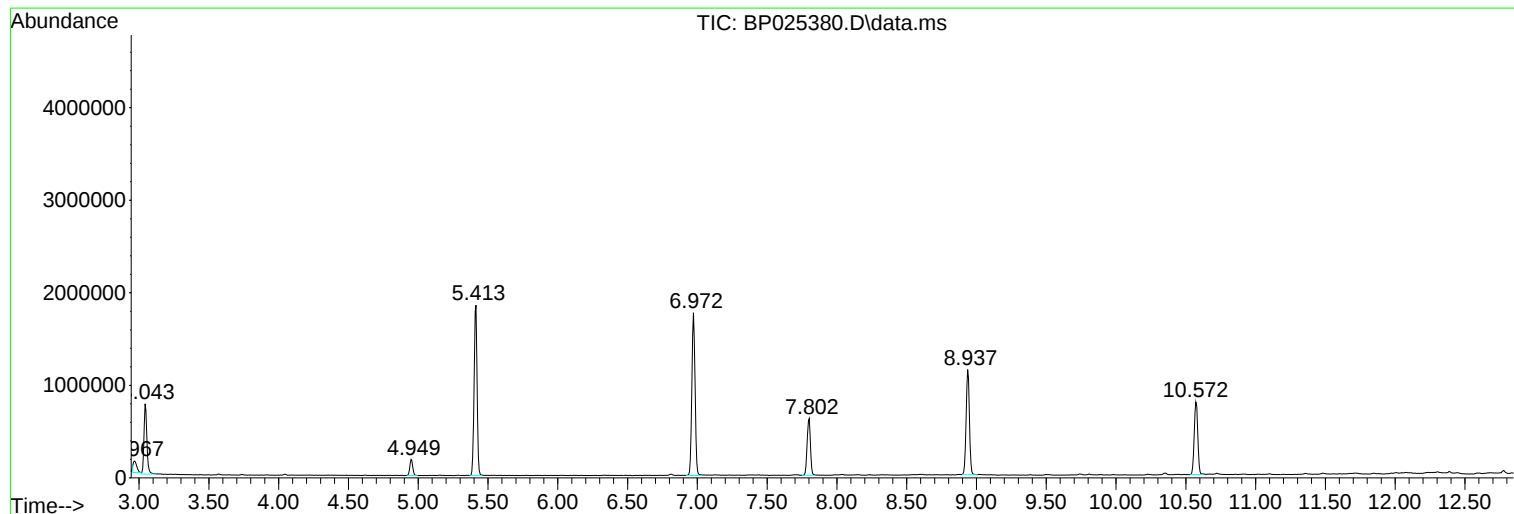
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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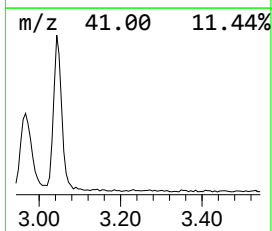
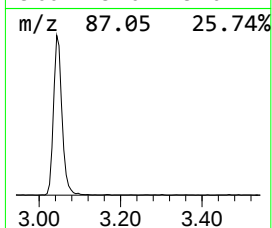
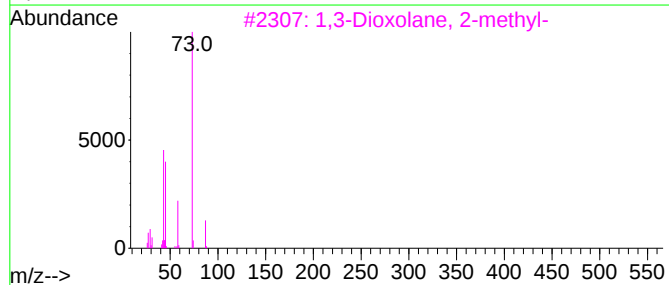
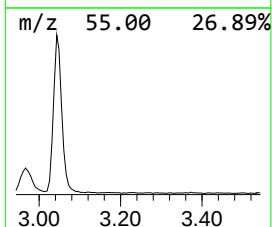
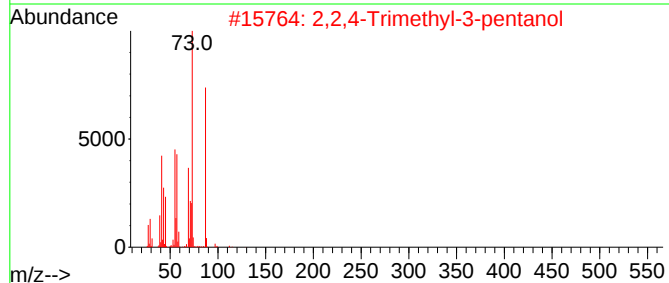
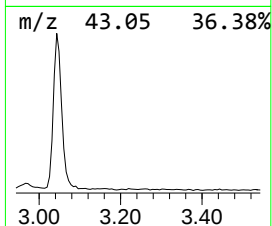
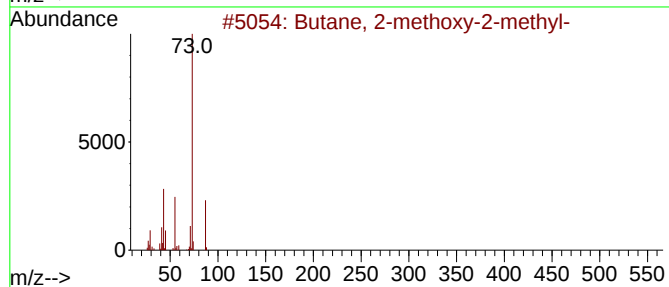
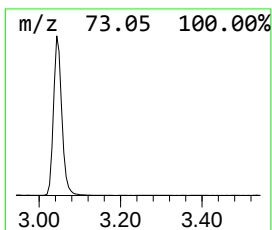
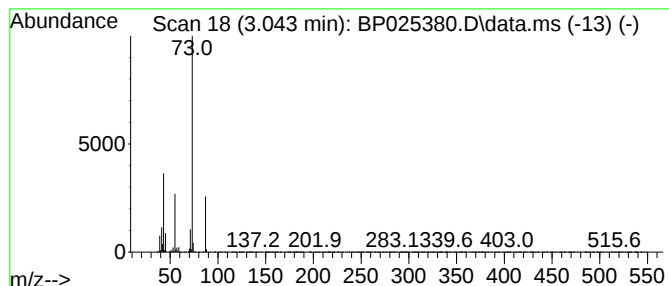
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.043	22.23 ng	1107100	1,4-Dichlorobenzene-d4	7.802

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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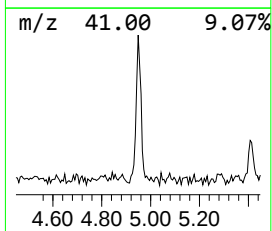
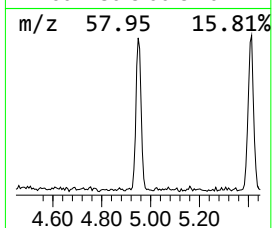
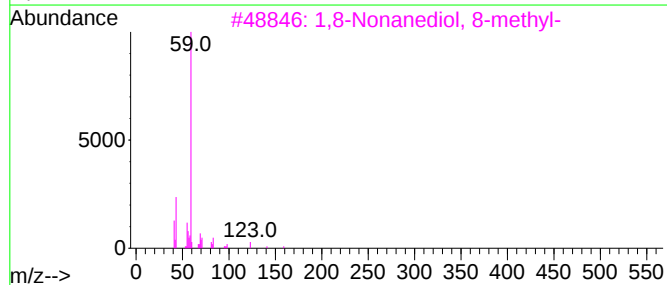
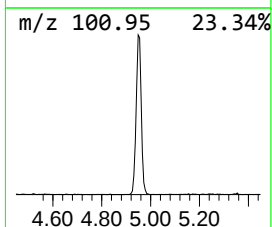
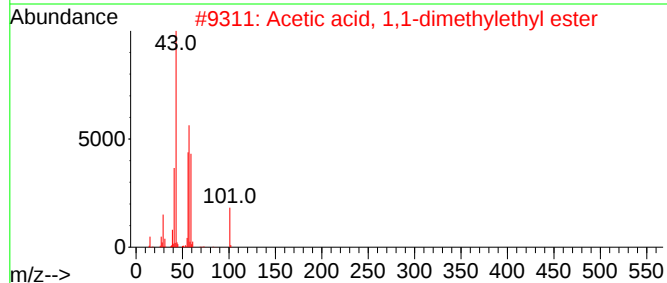
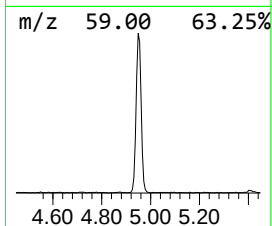
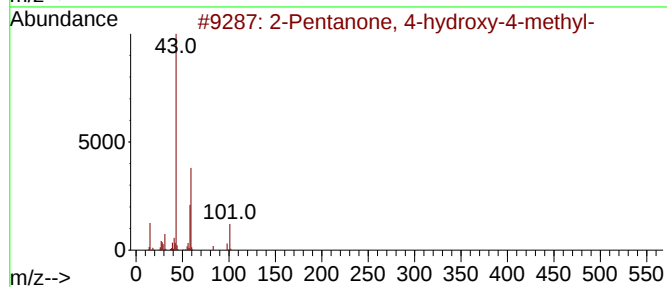
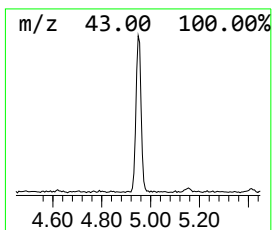
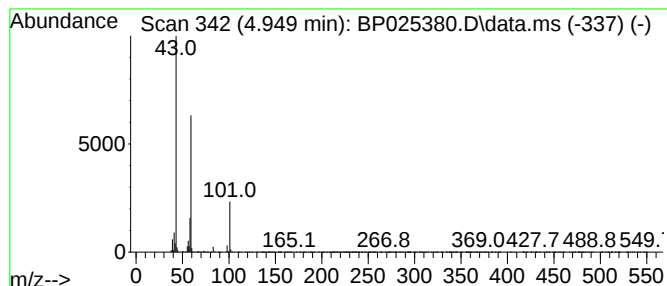
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.949	5.12 ng	254842	1,4-Dichlorobenzene-d4	7.802

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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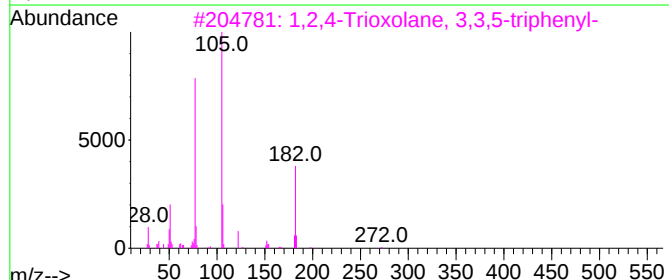
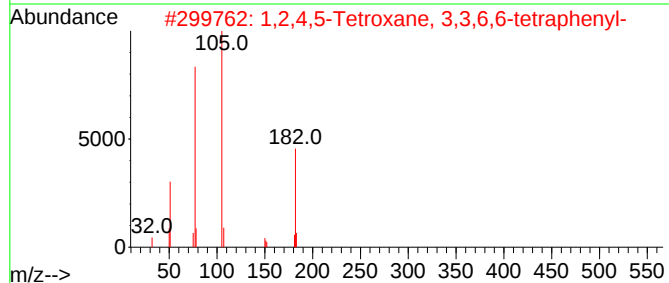
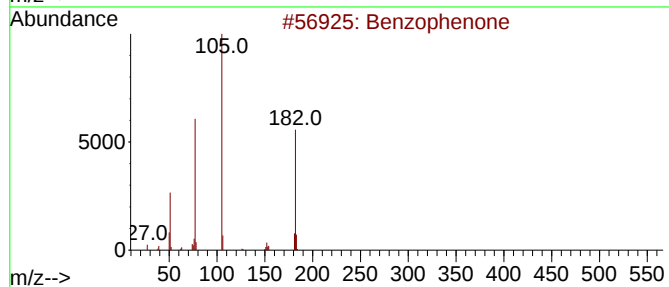
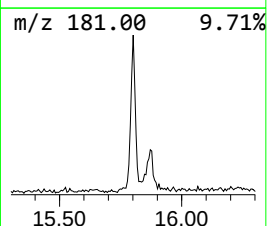
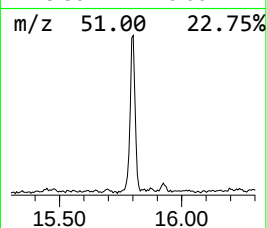
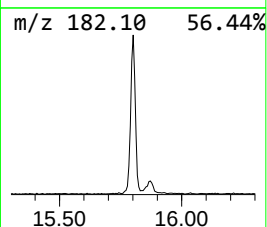
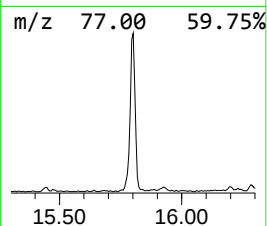
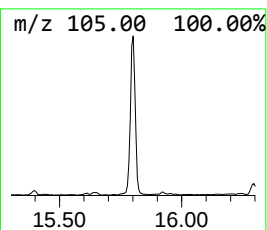
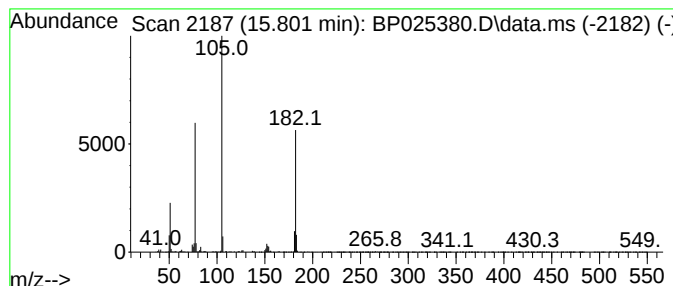
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.801	4.80 ng	429714	Acenaphthene-d10	14.419

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
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	64
4			Azobenzene	182	C12H10N2	000103-33-3	40
5			1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	30



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Instrument :
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ClientSampleId :
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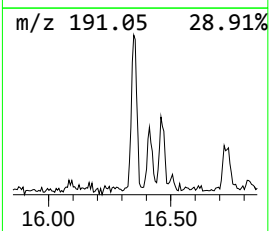
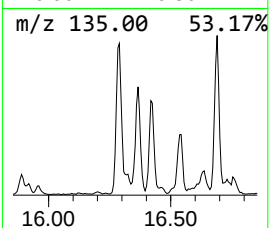
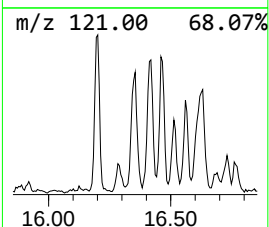
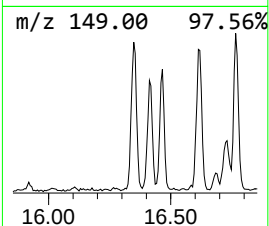
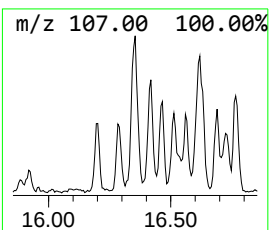
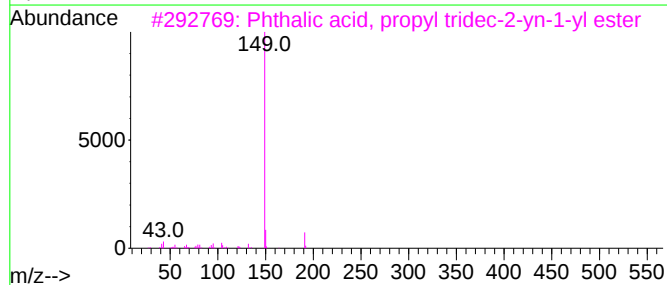
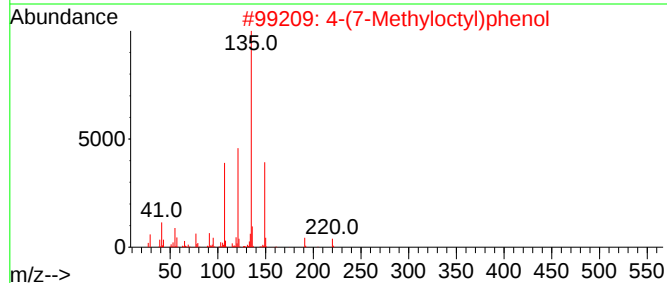
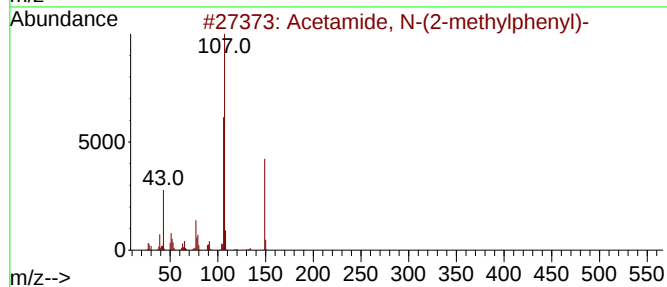
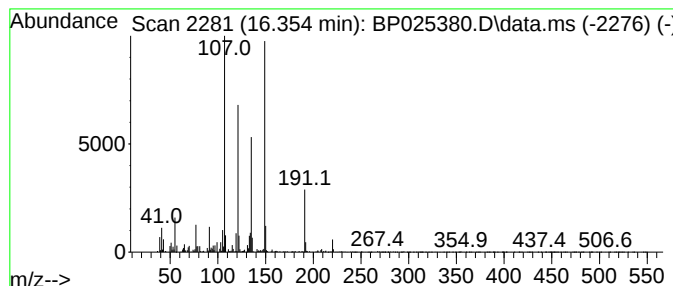
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Peak Number 5 unknown16.354 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	3.02 ng	306996	Phenanthrene-d10	17.225

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	43
2			4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	38
3			Phthalic acid, propyl tridec-2-y...	386	C24H34O4	1000315-43-6	35
4			Phthalic acid, 4-methoxyphenyl p...	314	C18H18O5	1000309-77-7	35
5			Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	35



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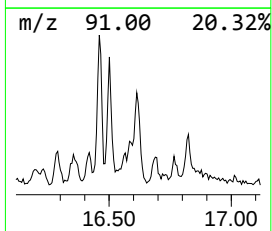
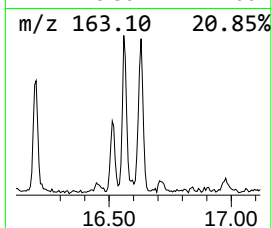
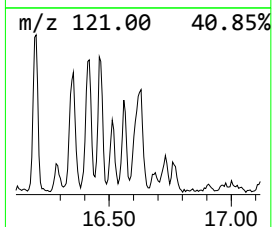
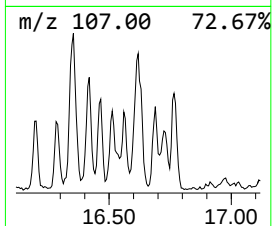
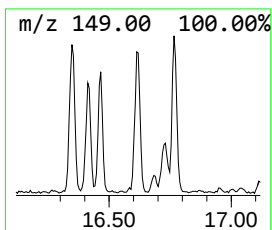
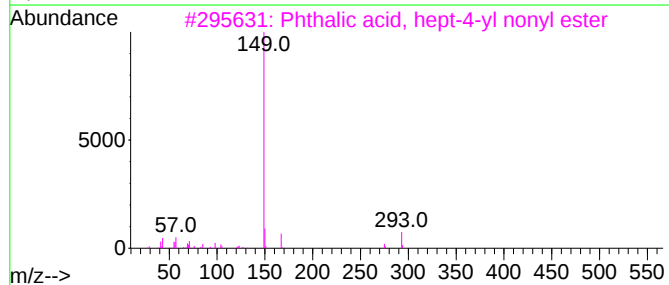
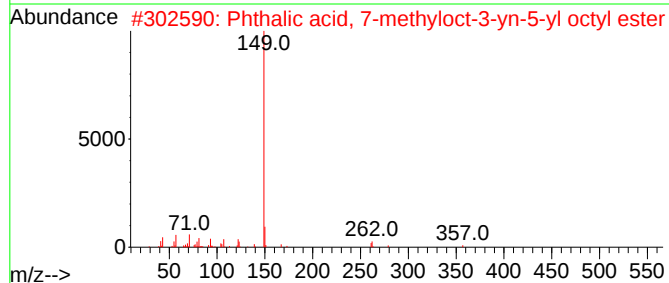
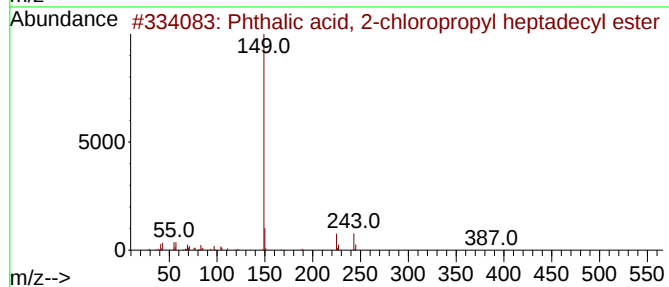
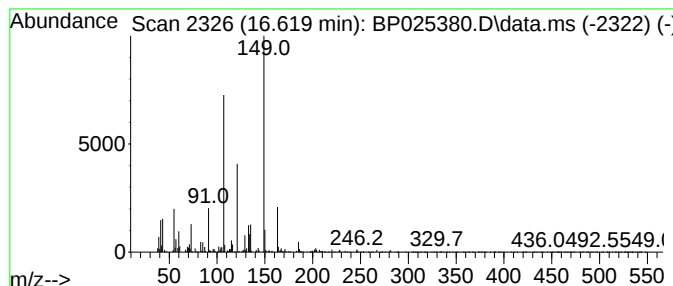
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown16.619 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.619	2.77 ng	281324	Phenanthrene-d10	17.225

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2-chloropropyl he...	480	C28H45ClO4	1000356-83-8	35
2			Phthalic acid, 7-methyloct-3-yn-...	400	C25H36O4	1000315-43-0	35
3			Phthalic acid, hept-4-yl nonyl e...	390	C24H38O4	1000356-79-0	35
4			Phthalic acid, butyl 5-methoxy-3...	336	C19H28O5	1000314-88-5	35
5			Phthalic acid, 5-methoxy-3-methy...	434	C26H42O5	1000314-89-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025380.D
Acq On : 13 Aug 2025 11:59
Operator : CG/JU
Sample : Q2820-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

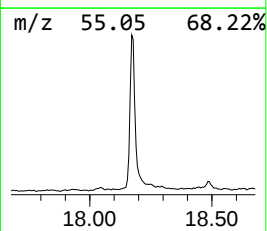
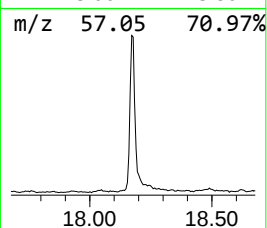
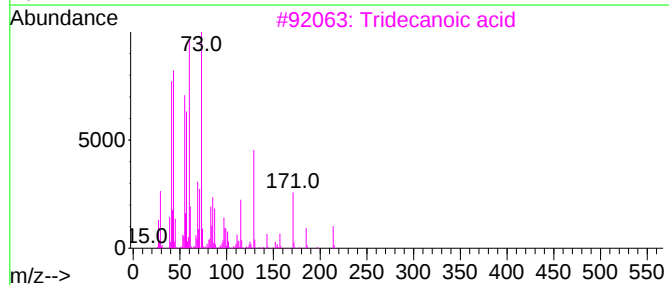
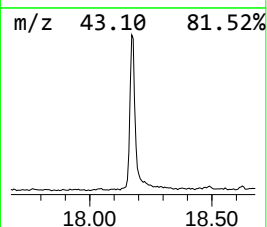
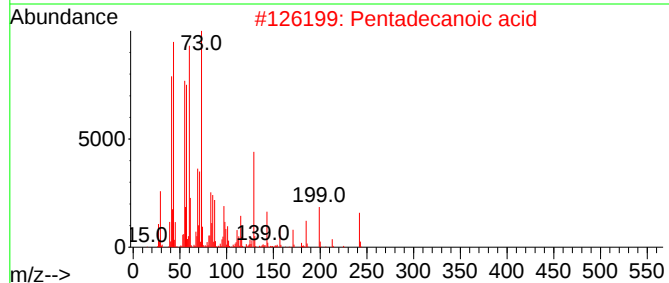
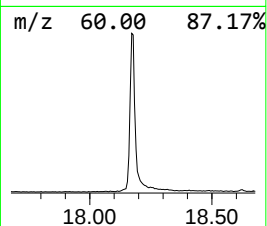
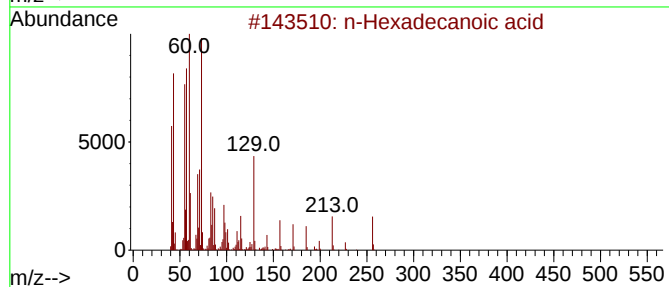
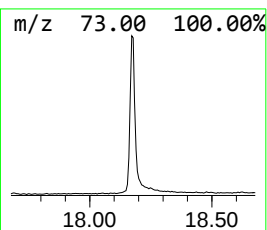
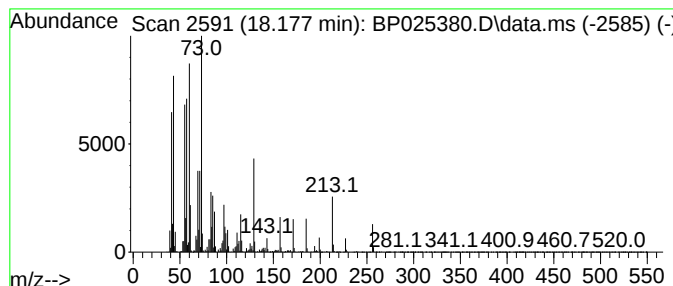
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ClientSampleId :
82H-W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
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 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.177	23.11 ng	2349220	Phenanthrene-d10		17.225	
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	91
3	Tridecanoic acid		214	C13H26O2	000638-53-9	89
4	n-Decanoic acid		172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025380.D
Acq On : 13 Aug 2025 11:59
Operator : CG/JU
Sample : Q2820-02
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ALS Vial : 5 Sample Multiplier: 1

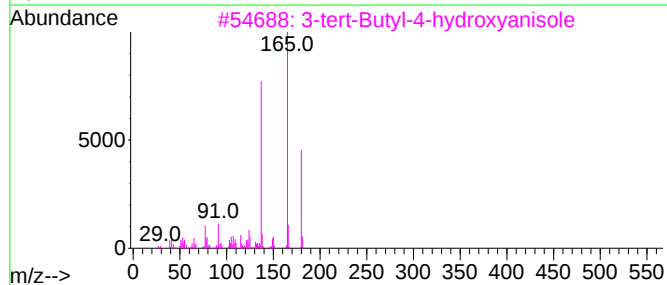
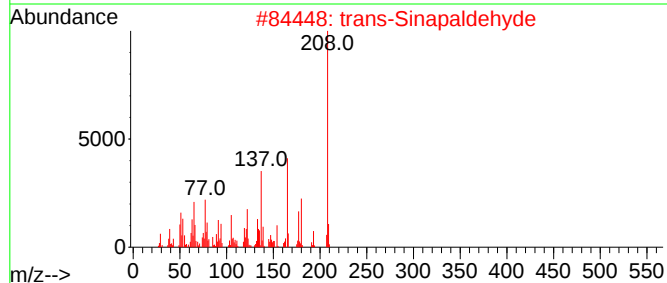
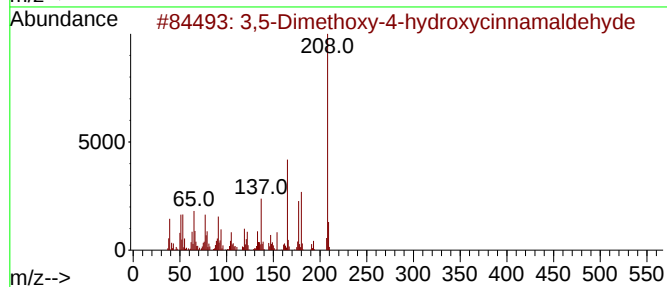
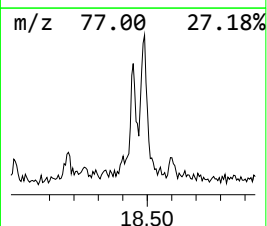
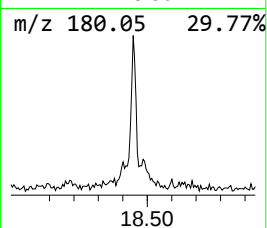
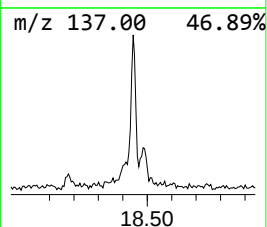
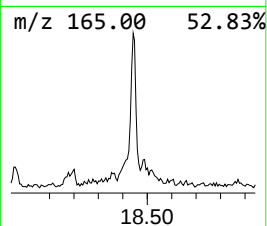
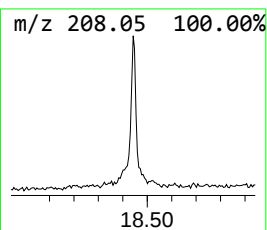
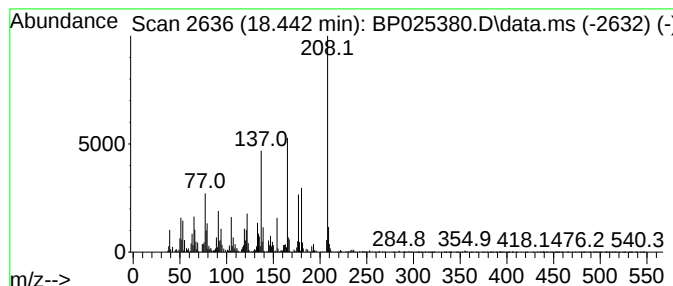
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.442	2.08 ng	211280	Phenanthrene-d10	17.225	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamal...	208	C11H12O4	087345-53-7	96
2	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	95
3	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	42
4	1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	41
5	4-(4-Fluoro-3-methylphenyl)-1,3-...	208	C10H9FN2S	003830-48-6	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025380.D
Acq On : 13 Aug 2025 11:59
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Sample : Q2820-02
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ClientSampleId :
82H-W

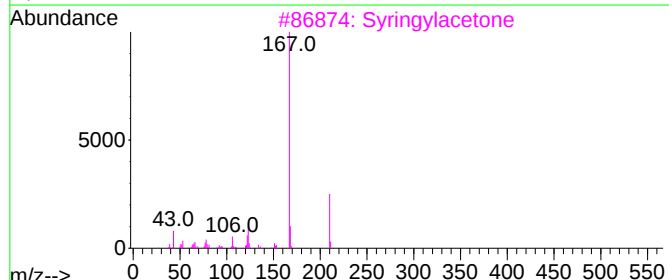
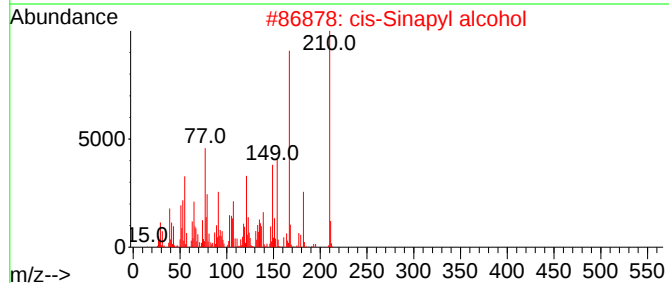
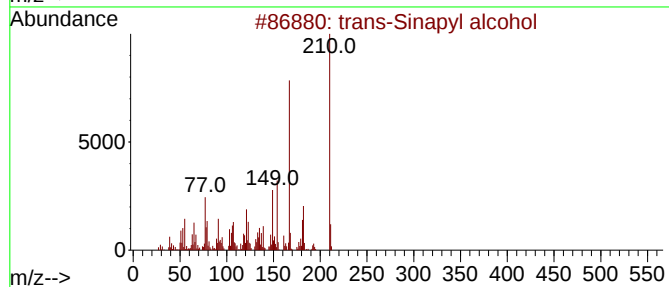
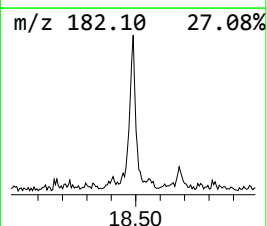
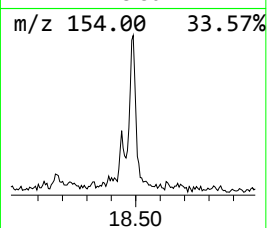
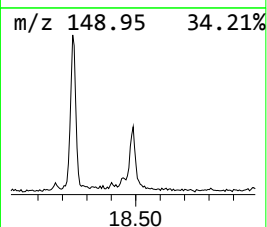
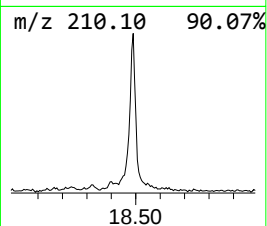
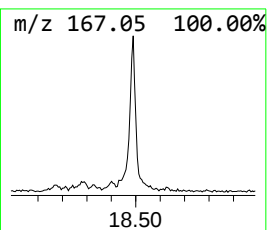
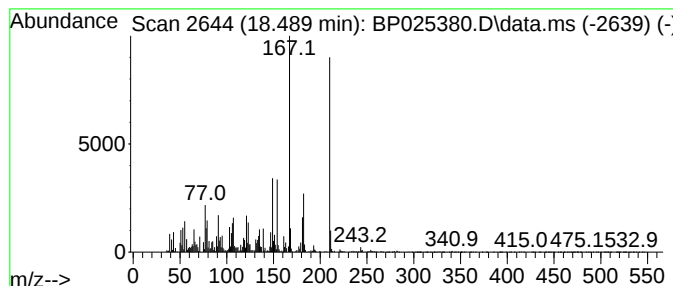
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 trans-Sinapyl alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	4.20 ng	427296	Phenanthrene-d10	17.225

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	93
2			cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	87
3			Syringylacetone	210	C11H14O4	019037-58-2	64
4			2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	52
5			Desaspidinol	210	C11H14O4	000437-72-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025380.D
Acq On : 13 Aug 2025 11:59
Operator : CG/JU
Sample : Q2820-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
82H-W

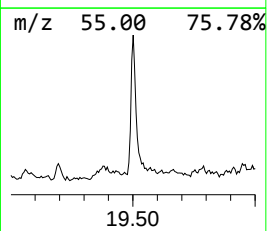
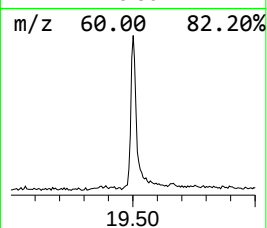
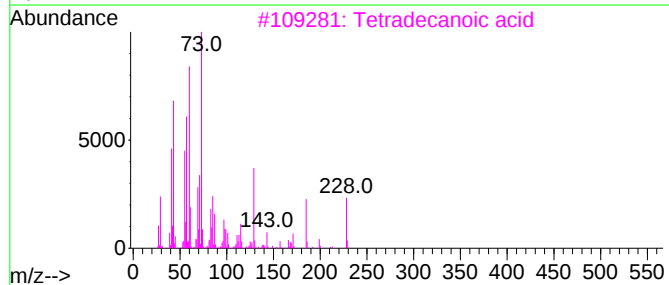
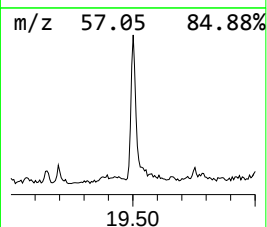
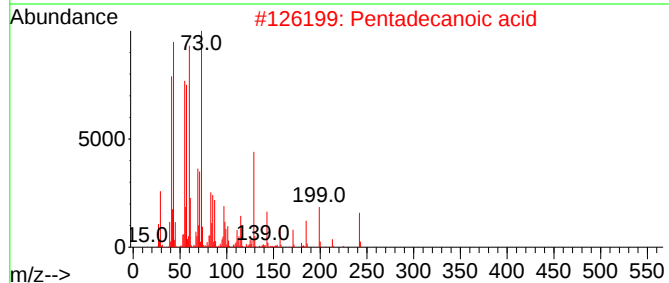
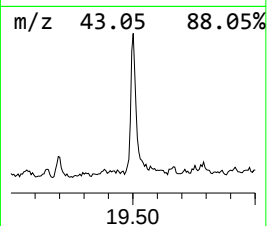
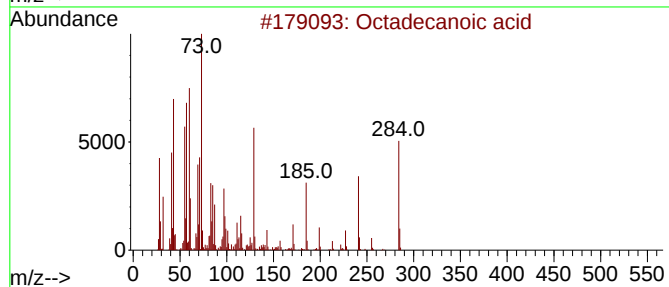
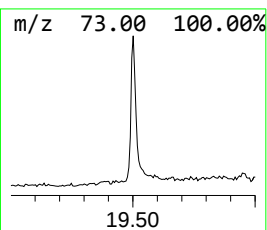
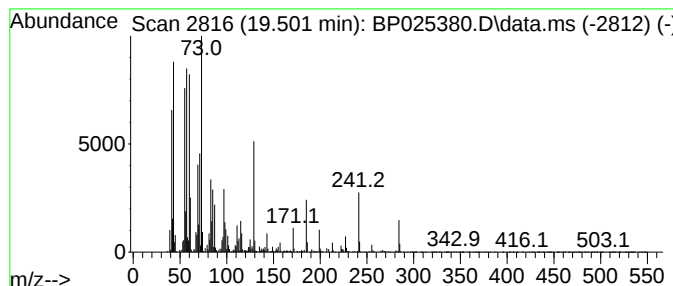
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.501	5.67 ng	688628	Chrysene-d12	21.677

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025380.D
Acq On : 13 Aug 2025 11:59
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Sample : Q2820-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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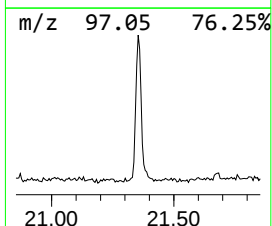
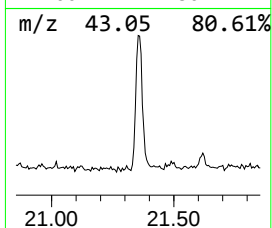
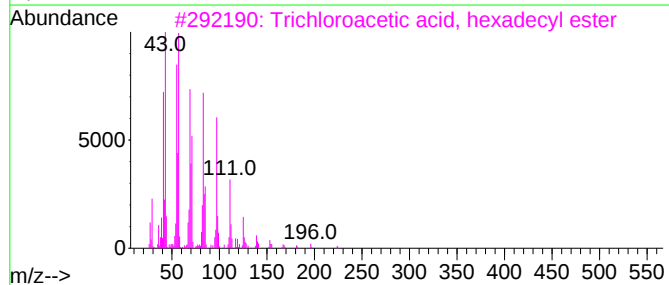
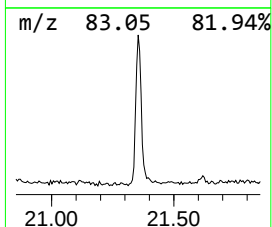
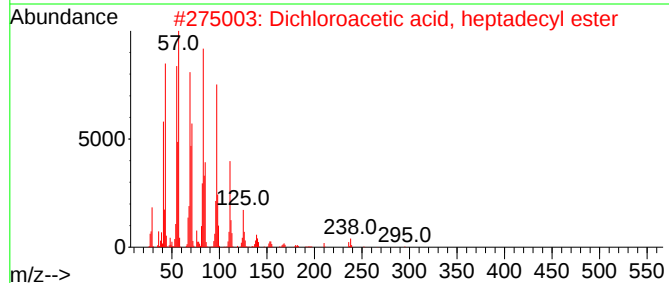
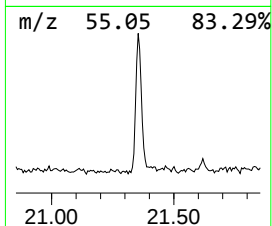
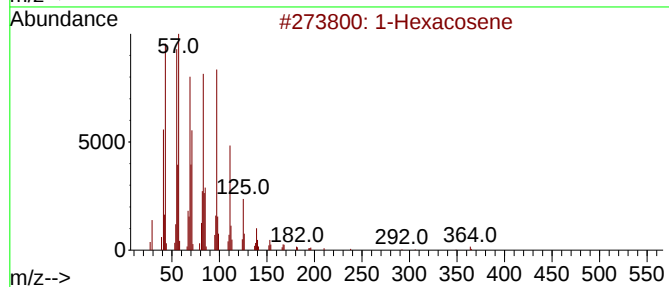
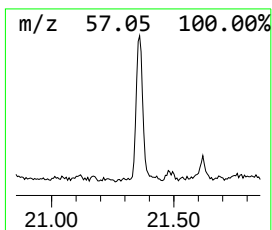
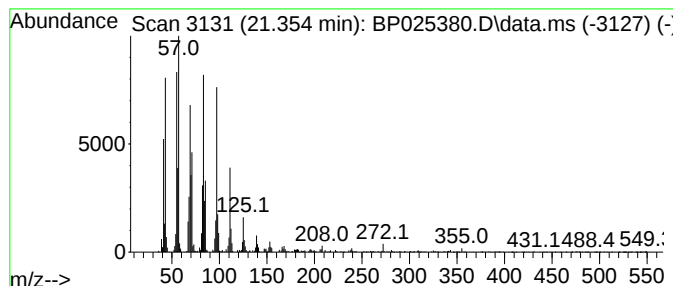
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.354	5.63 ng	683075	Chrysene-d12	21.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	95
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025380.D
Acq On : 13 Aug 2025 11:59
Operator : CG/JU
Sample : Q2820-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.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
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2-Pentanone, 4-...	4.949	5.1	ng	254842	1	7.802	996010	20.0
Benzophenone	15.801	4.8	ng	429714	3	14.419	1789280	20.0
unknown16.354	16.354	3.0	ng	306996	4	17.225	2032750	20.0
unknown16.619	16.619	2.8	ng	281324	4	17.225	2032750	20.0
n-Hexadecanoic ...	18.177	23.1	ng	2349220	4	17.225	2032750	20.0
3,5-Dimethoxy-4...	18.442	2.1	ng	211280	4	17.225	2032750	20.0
trans-Sinapyl a...	18.489	4.2	ng	427296	4	17.225	2032750	20.0
Octadecanoic acid	19.501	5.7	ng	688628	5	21.677	2428320	20.0
1-Hexacosene	21.354	5.6	ng	683075	5	21.677	2428320	20.0