

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
 Data File : BP024343.D
 Acq On : 18 Apr 2025 15:22
 Operator : RC/JU
 Sample : Q1822-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TW-WTS-06

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-BP041425.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	301	306	314	rBV	205235	287893	2.25%	0.386%
2	5.340	377	383	393	rBV	1588194	2332218	18.23%	3.124%
3	6.905	642	649	667	rBV	894718	1434931	11.22%	1.922%
4	7.722	781	788	796	rVB	842706	1328104	10.38%	1.779%
5	8.863	976	982	995	rVB	2110232	3459935	27.05%	4.634%
6	10.493	1251	1259	1269	rBV	1174783	1836803	14.36%	2.460%
7	10.863	1315	1322	1337	rBV	65112	182141	1.42%	0.244%
8	11.793	1469	1480	1483	rBV3	46902	144694	1.13%	0.194%
9	12.193	1532	1548	1556	rBV	2468026	8876469	69.39%	11.889%
10	12.963	1672	1679	1688	rBV	5435985	7554778	59.06%	10.119%
11	13.163	1706	1713	1723	rBV	280006	745501	5.83%	0.998%
12	13.251	1723	1728	1734	rVV2	206845	392556	3.07%	0.526%
13	13.322	1734	1740	1769	rVB	368952	1202176	9.40%	1.610%
14	14.351	1908	1915	1924	rVB	1600053	2306822	18.03%	3.090%
15	15.187	2042	2057	2070	rBV	372927	714312	5.58%	0.957%
16	15.869	2166	2173	2192	rBV	4391175	6578749	51.43%	8.811%
17	16.463	2270	2274	2281	rBV	71757	146028	1.14%	0.196%
18	16.663	2299	2308	2327	rBV	3679501	6125631	47.88%	8.204%
19	16.798	2327	2331	2341	rVB2	78804	151743	1.19%	0.203%
20	17.151	2385	2391	2397	rBV2	1750577	2641464	20.65%	3.538%
21	17.210	2397	2401	2407	rVV	165389	233704	1.83%	0.313%
22	17.292	2411	2415	2421	rVV	146398	208647	1.63%	0.279%
23	17.392	2427	2432	2440	rBV	181131	295310	2.31%	0.396%
24	18.092	2545	2551	2559	rBV	1445776	2041647	15.96%	2.735%
25	18.163	2560	2563	2570	rVB	162020	234953	1.84%	0.315%
26	19.422	2772	2777	2794	rBV	899389	1566802	12.25%	2.099%
27	19.651	2812	2816	2822	rBV	86850	150996	1.18%	0.202%
28	19.875	2848	2854	2864	rBV	9713148	12792588	100.00%	17.134%
29	20.686	2989	2992	2998	rBV	316399	404156	3.16%	0.541%
30	21.592	3140	3146	3157	rVB2	2260798	3536484	27.64%	4.737%
31	23.227	3420	3424	3431	rVB	172806	312989	2.45%	0.419%
32	24.086	3565	3570	3580	rVB	252774	520563	4.07%	0.697%
33	24.945	3707	3716	3730	rVB	1593834	3920499	30.65%	5.251%

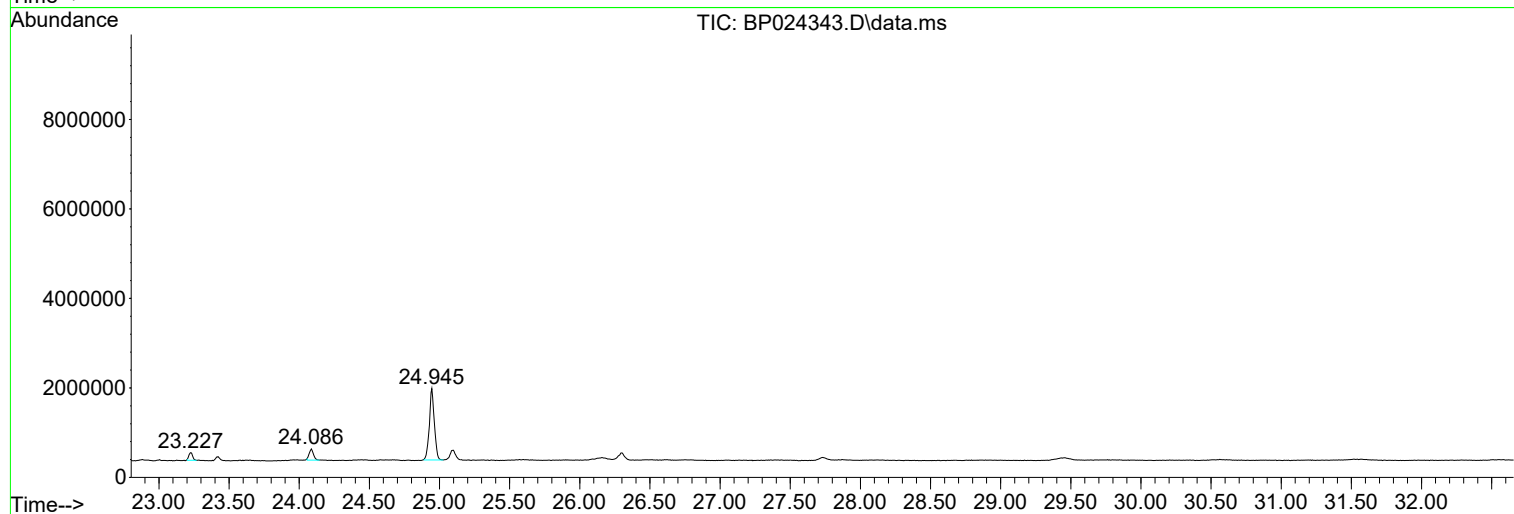
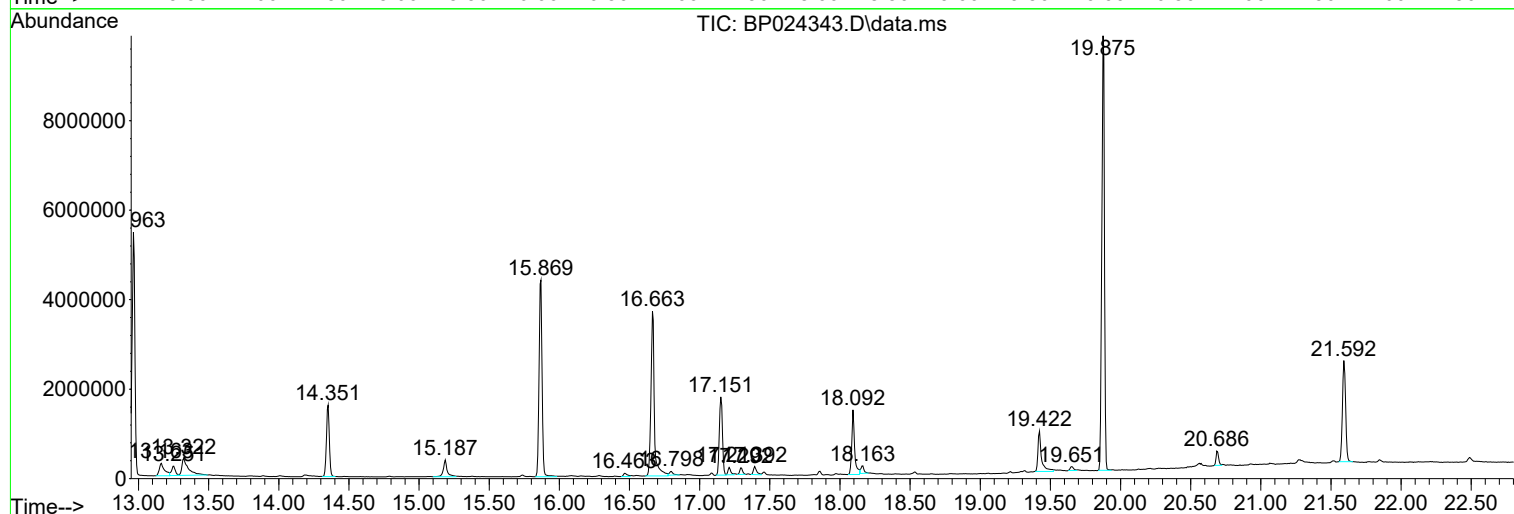
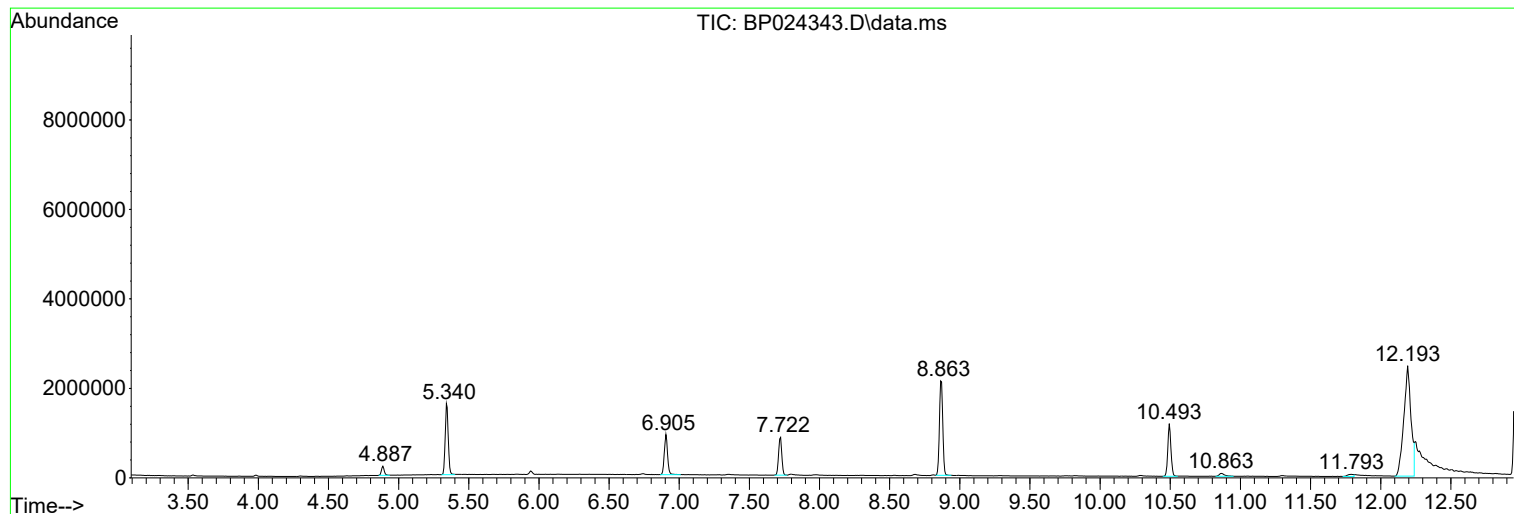
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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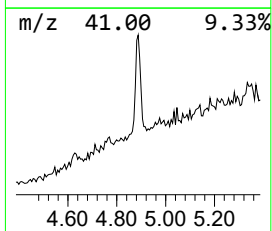
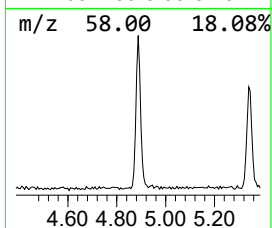
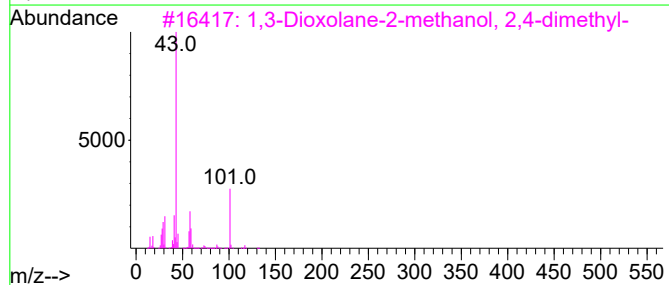
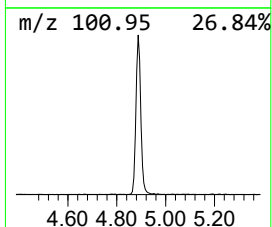
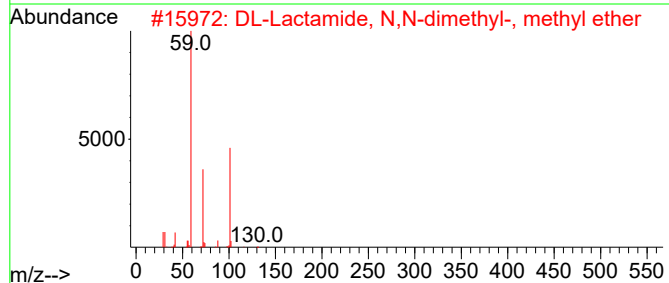
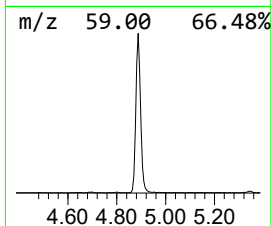
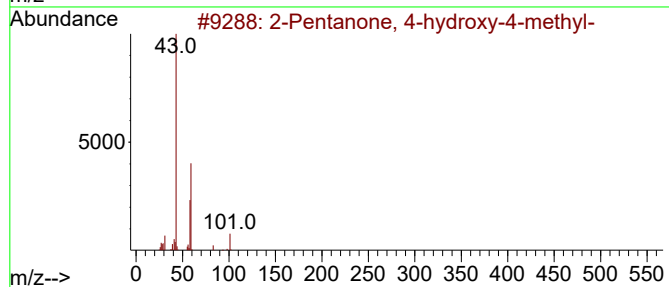
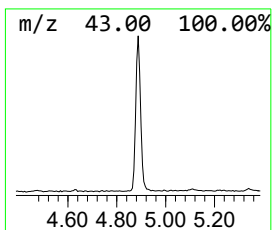
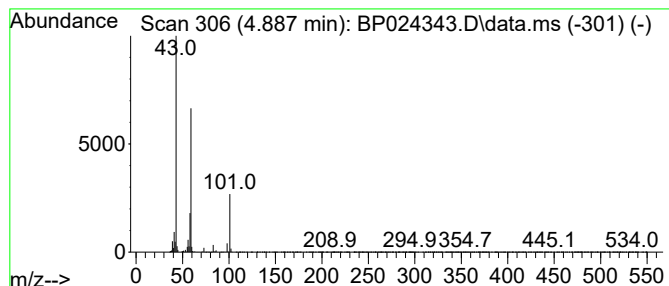
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	4.34 ng	287893	1,4-Dichlorobenzene-d4	7.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	33
3			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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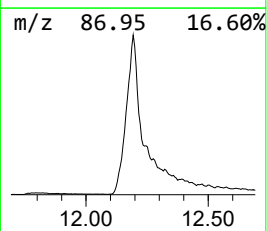
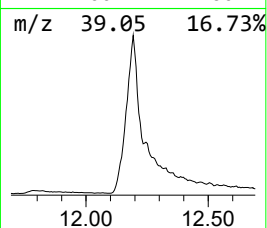
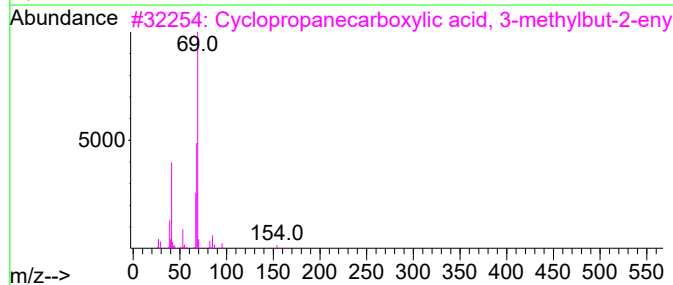
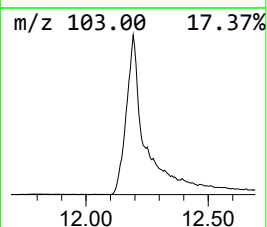
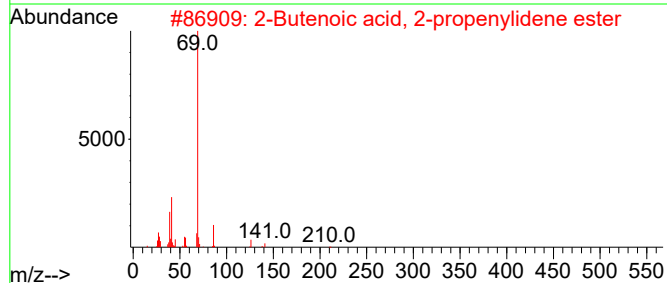
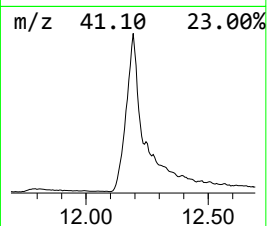
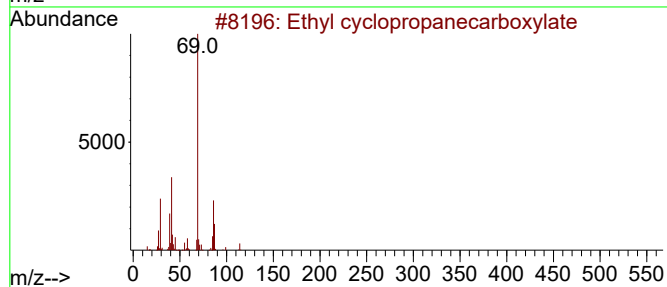
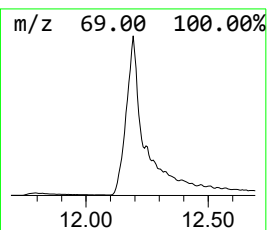
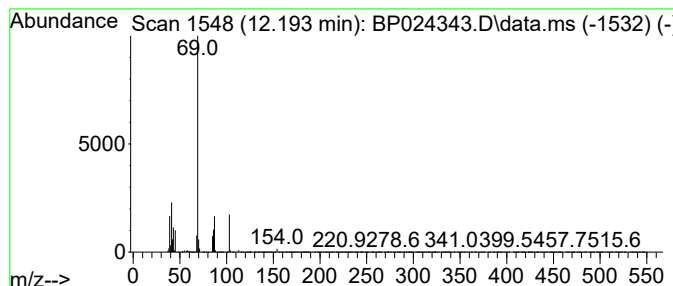
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethyl cyclopropanecarboxylate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.193	96.65 ng	8876470	Naphthalene-d8	10.493

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	56
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
3			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9
4			2-Hydroxyethyl methacrylate	130	C6H10O3	000868-77-9	9
5			Vinyl crotonate	112	C6H8O2	014861-06-4	9



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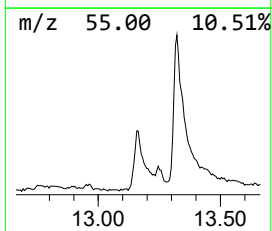
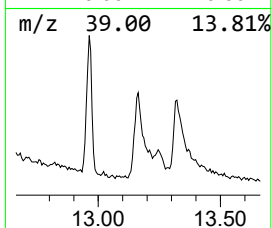
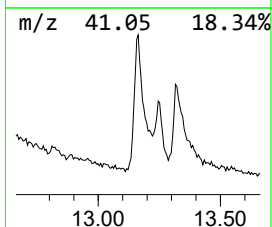
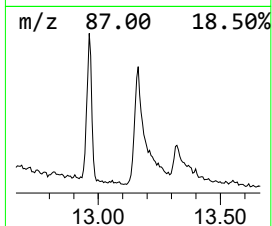
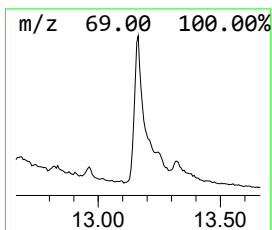
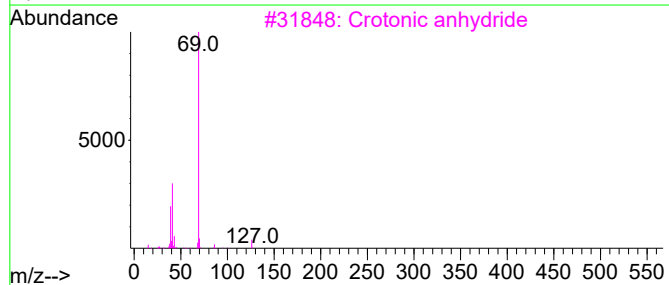
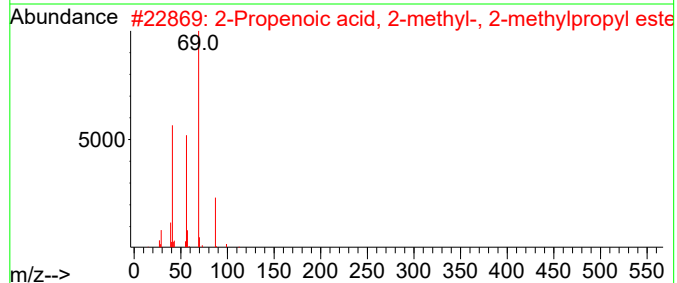
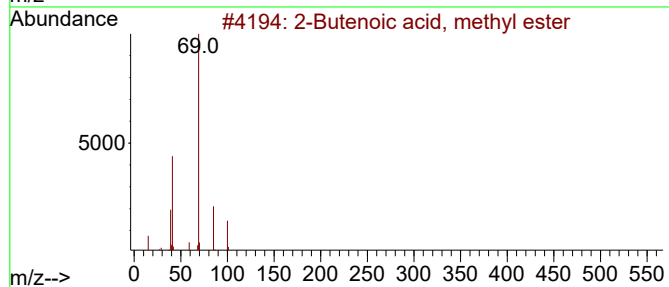
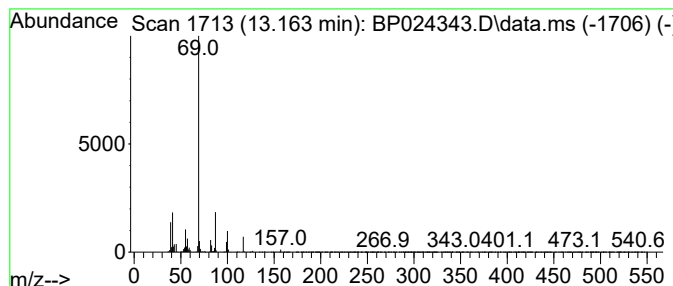
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown13.163 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	6.46 ng	745501	Acenaphthene-d10	14.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenoic acid, methyl ester	100	C5H8O2	018707-60-3	45
2			2-Propenoic acid, 2-methyl-, 2-m...	142	C8H14O2	000097-86-9	45
3			Crotonic anhydride	154	C8H10O3	000623-68-7	40
4			4-Hexen-3-one	98	C6H10O	002497-21-4	40
5			2-Butenoic acid, butyl ester	142	C8H14O2	007299-91-4	38



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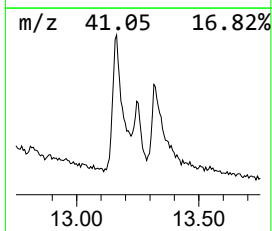
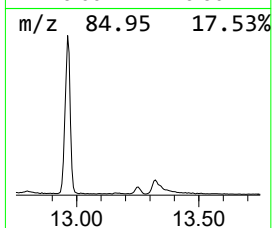
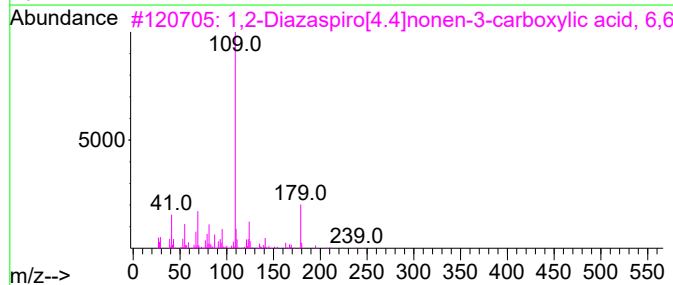
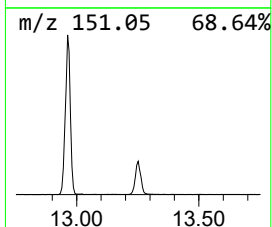
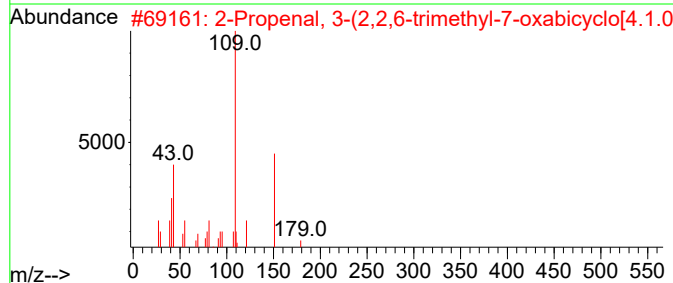
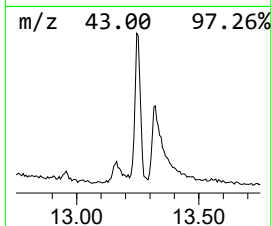
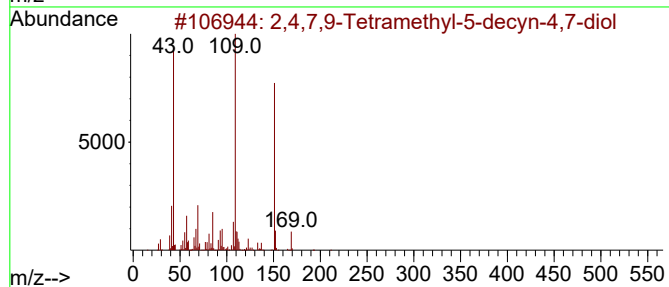
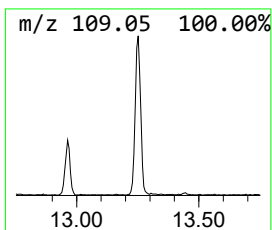
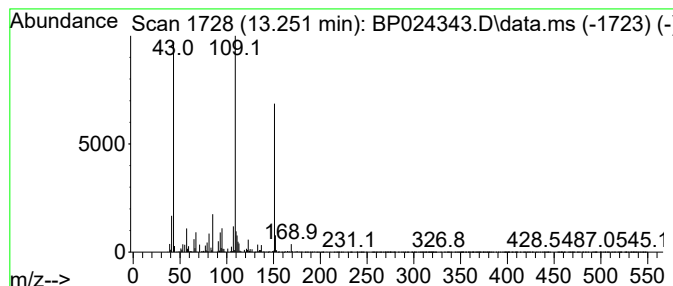
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Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	3.40 ng	392556	Acenaphthene-d10	14.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	72		
3	1,2-Diazaspiro[4.4]nonen-3-carbo...	238	C13H22N2O2	1000164-25-8	47		
4	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	46		
5	Cyclopentanol, 1-(methylenecyclo...	138	C9H14O	086951-58-8	43		



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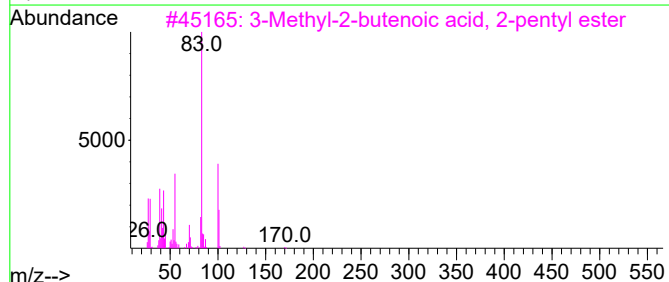
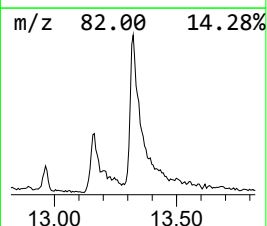
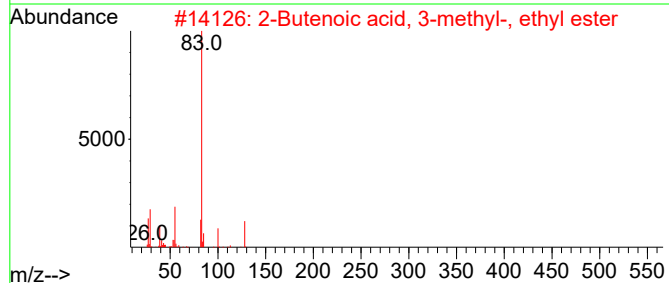
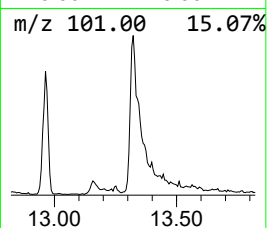
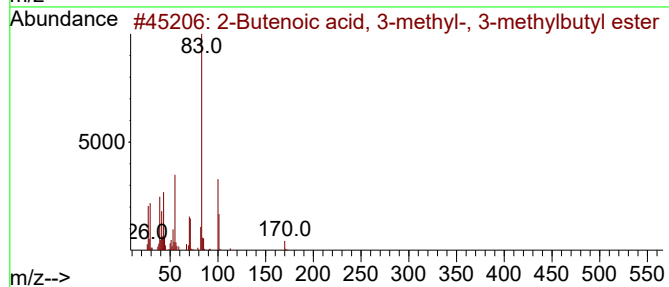
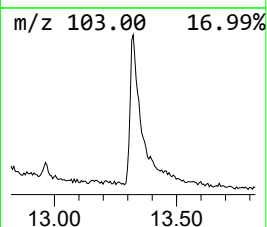
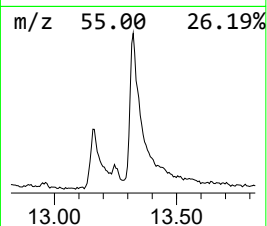
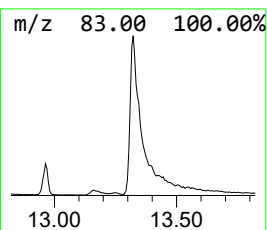
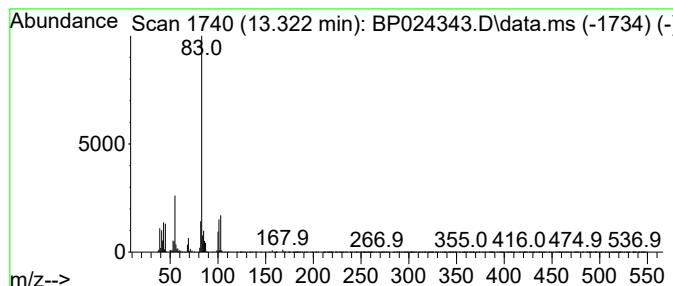
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Peak Number 5 2-Butenoic acid, 3-methyl-,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.322	10.42 ng	1202180	Acenaphthene-d10	14.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenoic acid, 3-methyl-, 3-me...	170	C10H18O2	056922-73-7	59
2			2-Butenoic acid, 3-methyl-, ethy...	128	C7H12O2	000638-10-8	59
3			3-Methyl-2-butenic acid, 2-pent...	170	C10H18O2	150462-84-3	59
4			3-Methylbutan-2-yl (E)-2-methylb...	170	C10H18O2	1000373-73-4	53
5			Oxalic acid, cyclohexyl undecyl ...	326	C19H34O4	1000309-31-3	47



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-WTS-06

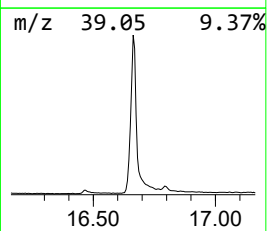
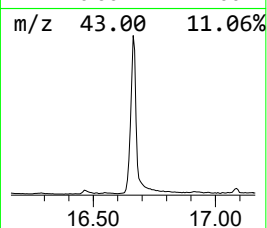
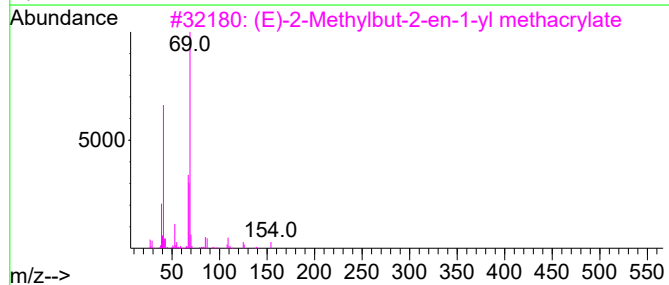
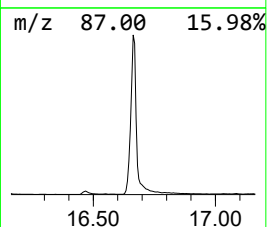
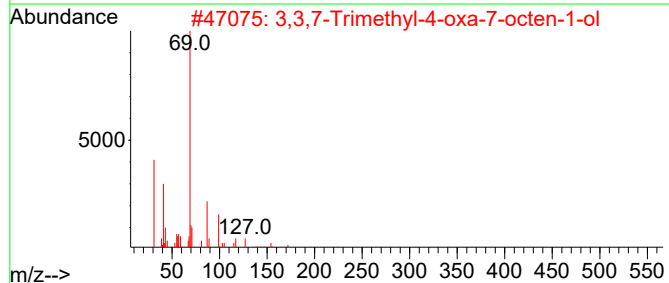
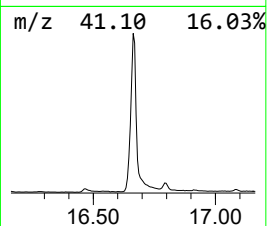
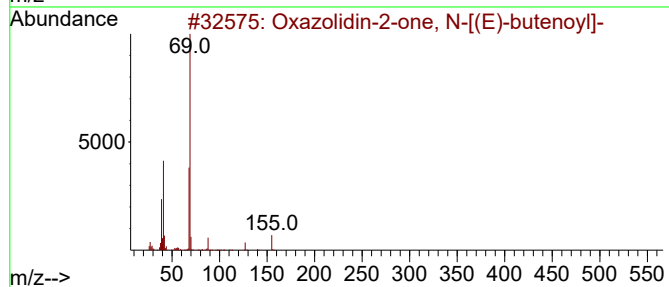
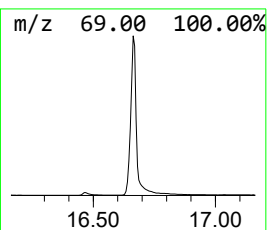
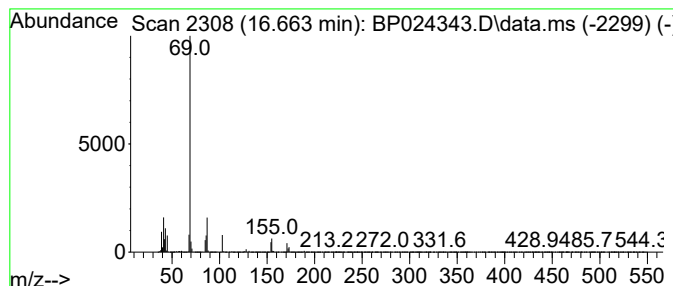
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.663 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.663	46.38 ng	6125630	Phenanthrene-d10	17.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1010156-45-5	40
2			3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	39
3			(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	38
4			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36
5			Cyclopropanecarboxylic acid, 2-m...	170	C10H18O2	1000354-65-8	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024343.D
Acq On : 18 Apr 2025 15:22
Operator : RC/JU
Sample : Q1822-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

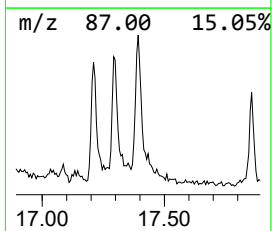
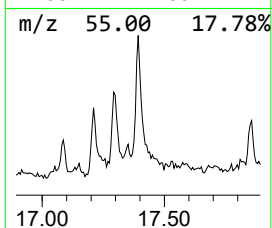
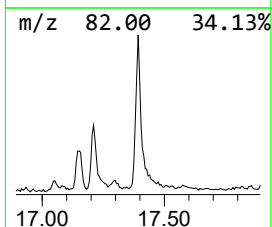
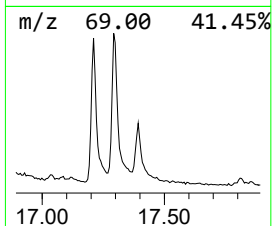
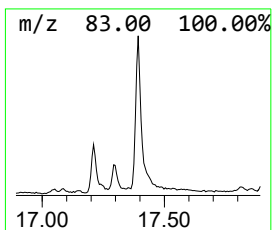
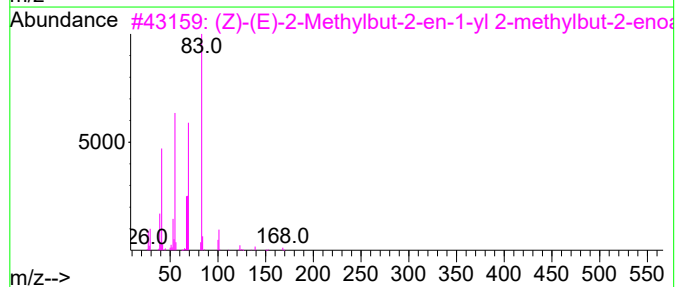
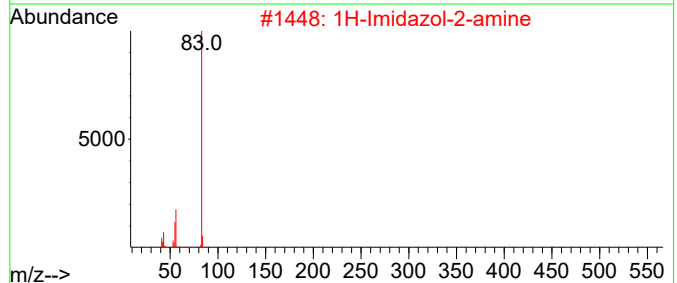
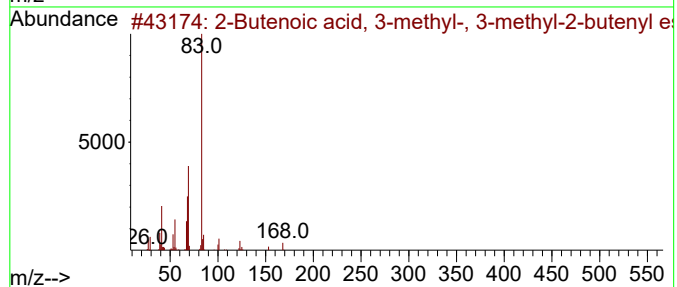
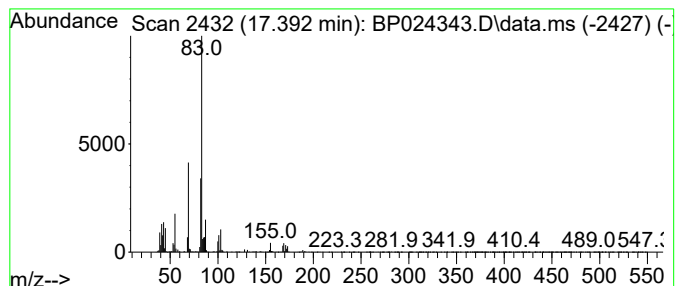
Instrument :
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ClientSampleId :
TW-WTS-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.392 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.392	2.24 ng	295310	Phenanthrene-d10	17.151	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 3-methyl-, 3-me...	168	C10H16O2	072779-06-7	49
2	1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	46
3	(Z)-(E)-2-Methylbut-2-en-1-yl 2-...	168	C10H16O2	090358-41-1	38
4	3-Methyl-2-butenic acid, 2-pent...	170	C10H18O2	150462-84-3	38
5	Penten-3-yl angelate, 1-	168	C10H16O2	1000383-59-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024343.D
Acq On : 18 Apr 2025 15:22
Operator : RC/JU
Sample : Q1822-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-WTS-06

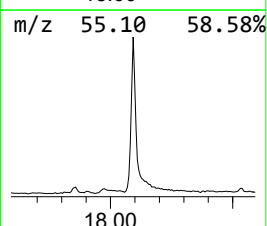
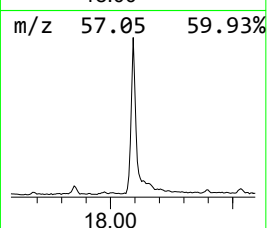
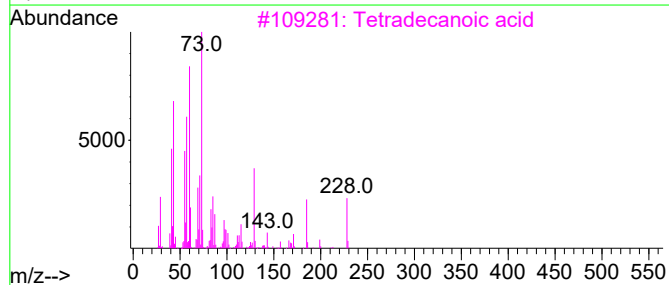
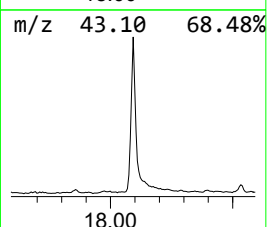
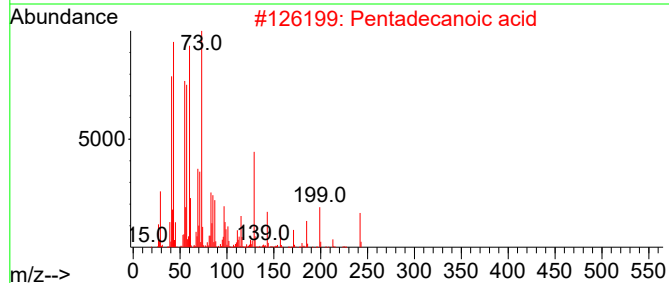
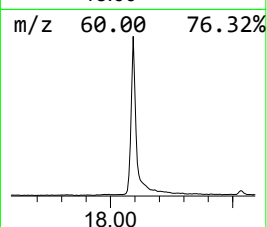
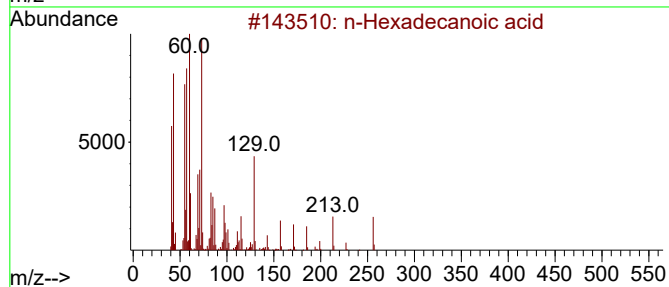
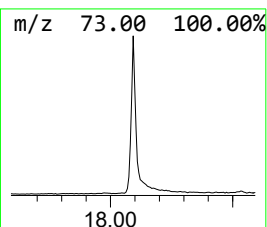
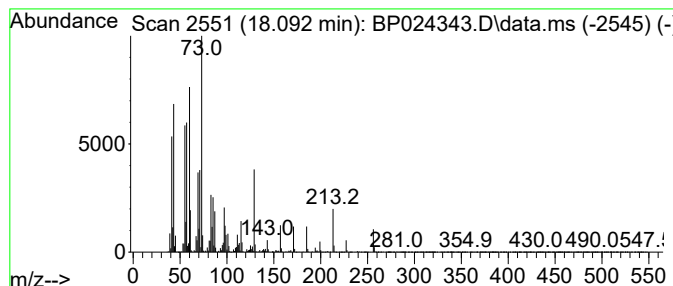
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	15.46 ng	2041650	Phenanthrene-d10	17.151

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	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024343.D
Acq On : 18 Apr 2025 15:22
Operator : RC/JU
Sample : Q1822-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-WTS-06

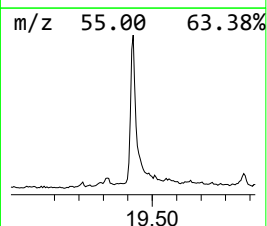
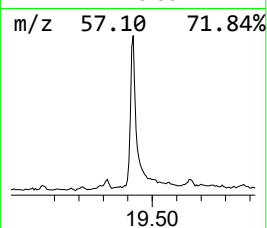
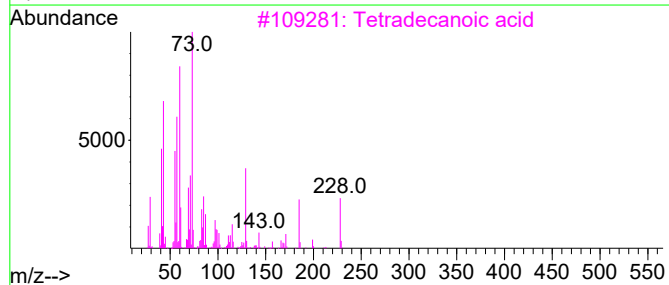
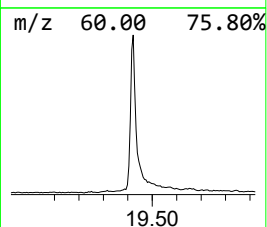
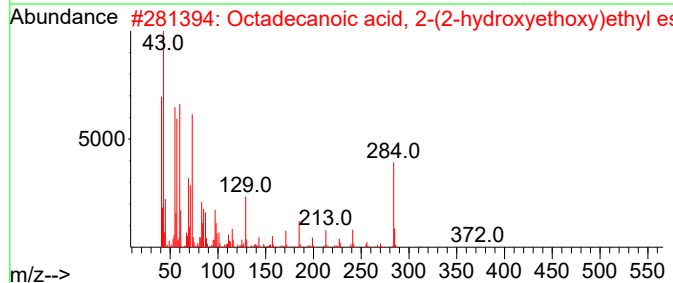
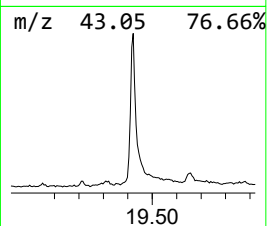
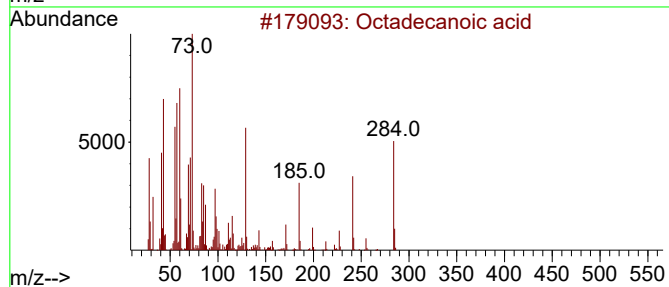
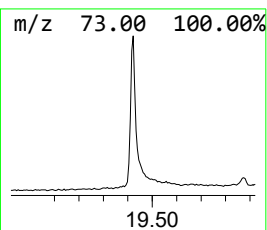
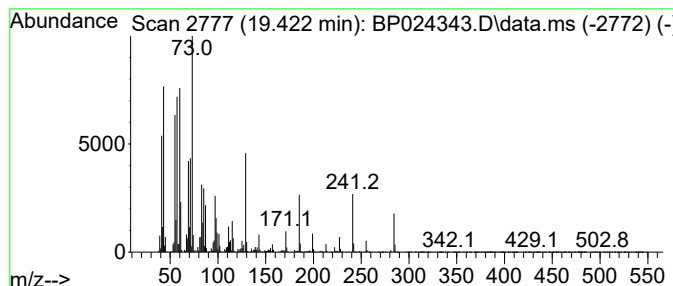
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	8.86 ng	1566800	Chrysene-d12	21.592

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	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024343.D
Acq On : 18 Apr 2025 15:22
Operator : RC/JU
Sample : Q1822-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-WTS-06

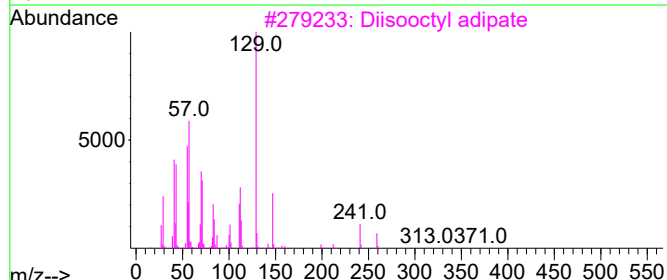
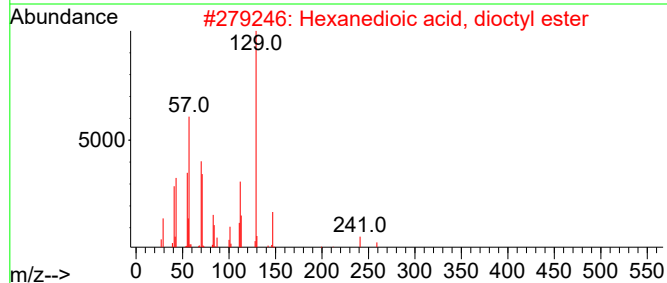
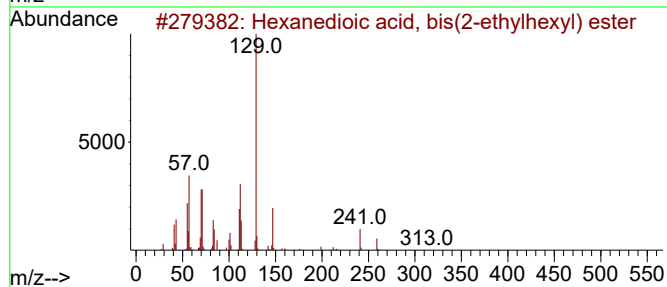
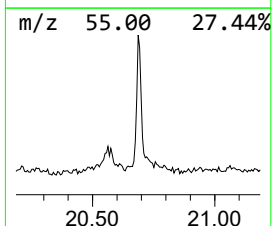
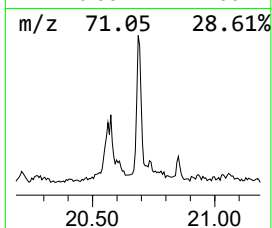
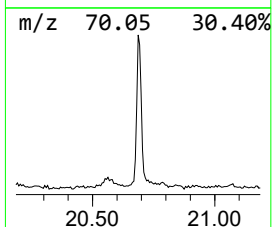
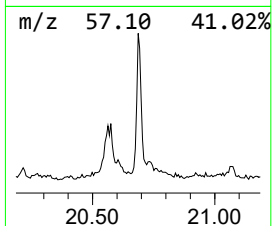
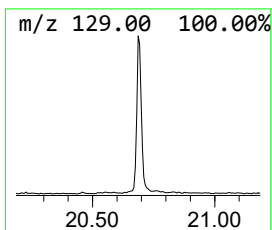
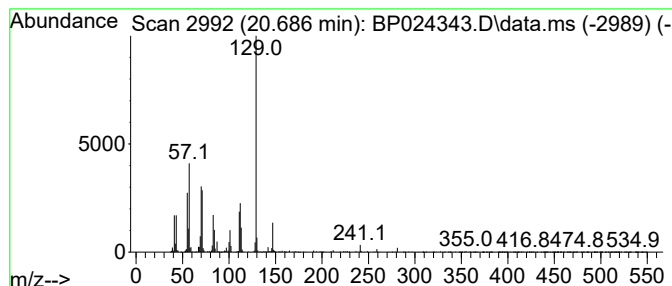
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexanedioic acid, bis(2-eth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.686	2.29 ng	404156	Chrysene-d12	21.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	91
3			Diisooctyl adipate	370	C22H42O4	001330-86-5	60
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58
5			Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024343.D
Acq On : 18 Apr 2025 15:22
Operator : RC/JU
Sample : Q1822-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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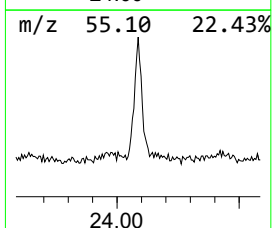
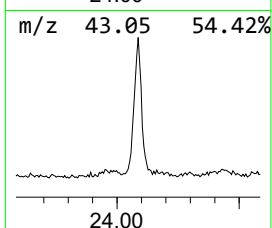
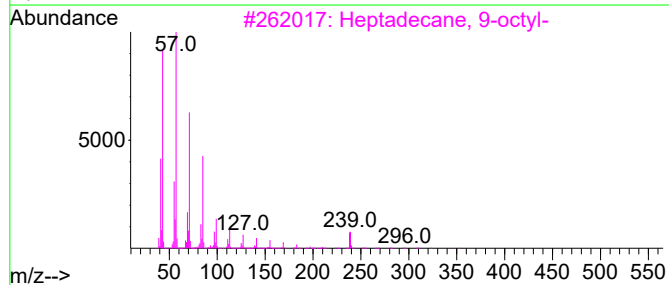
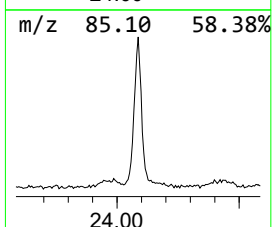
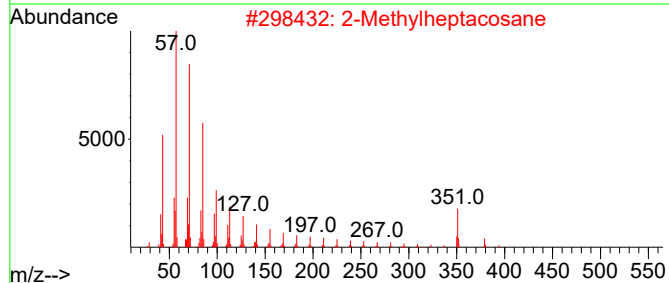
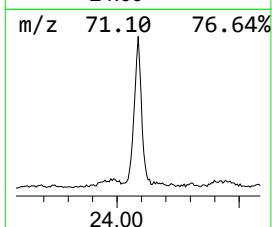
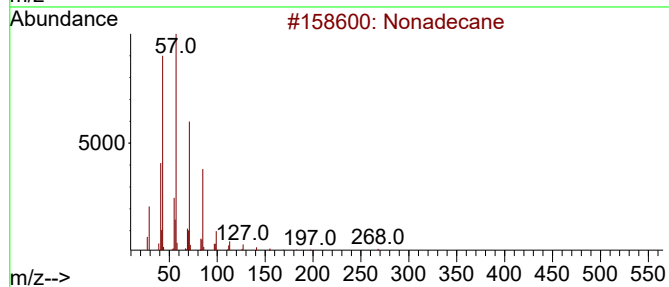
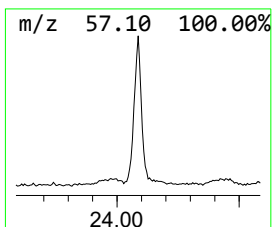
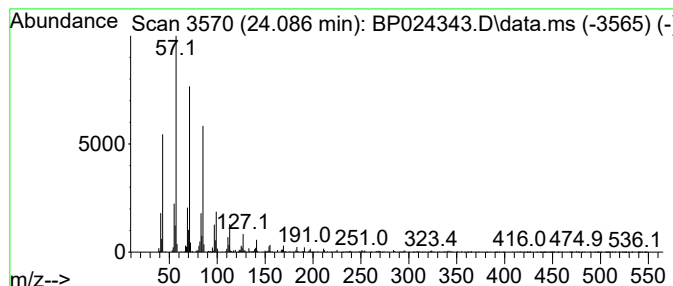
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.086	2.66 ng	520563	Perylene-d12	24.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	95
2		2-Methylheptacosane	394	C28H58	001561-00-8	94
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041825\
Data File : BP024343.D
Acq On : 18 Apr 2025 15:22
Operator : RC/JU
Sample : Q1822-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-WTS-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.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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Ethyl cycloprop...	12.193	96.7	ng	8876470	2	10.493	1836800	20.0
unknown13.163	13.163	6.5	ng	745501	3	14.351	2306820	20.0
2,4,7,9-Tetrame...	13.251	3.4	ng	392556	3	14.351	2306820	20.0
2-Butenoic acid...	13.322	10.4	ng	1202180	3	14.351	2306820	20.0
unknown16.663	16.663	46.4	ng	6125630	4	17.151	2641460	20.0
unknown17.392	17.392	2.2	ng	295310	4	17.151	2641460	20.0
n-Hexadecanoic ...	18.092	15.5	ng	2041650	4	17.151	2641460	20.0
Octadecanoic acid	19.422	8.9	ng	1566800	5	21.592	3536480	20.0
Hexanedioic aci...	20.686	2.3	ng	404156	5	21.592	3536480	20.0
Nonadecane	24.086	2.7	ng	520563	6	24.945	3920500	20.0