

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082625\
 Data File : BP025592.D
 Acq On : 26 Aug 2025 19:22
 Operator : CG/JU
 Sample : Q2947-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 235

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-BP081425.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.031	11	16	21	rBV	1146957	1515340	21.90%	3.392%
2	4.943	332	341	350	rBV	498295	734711	10.62%	1.645%
3	5.408	413	420	436	rBV	2736896	4129520	59.68%	9.244%
4	6.972	676	686	700	rBV	2602435	4389959	63.44%	9.827%
5	7.778	816	823	829	rBV	950145	1466098	21.19%	3.282%
6	8.919	1008	1017	1026	rBV	1773226	2993308	43.26%	6.701%
7	10.549	1287	1294	1300	rVB	1178829	1926683	27.84%	4.313%
8	12.996	1704	1710	1722	rBV	4440255	6919791	100.00%	15.490%
9	13.160	1733	1738	1745	rBV2	234282	506385	7.32%	1.134%
10	13.813	1844	1849	1855	rBV	267813	440154	6.36%	0.985%
11	13.925	1864	1868	1876	rVB2	314520	495798	7.16%	1.110%
12	14.043	1884	1888	1892	rBV	619042	828238	11.97%	1.854%
13	14.131	1896	1903	1907	rVV4	306384	705381	10.19%	1.579%
14	14.184	1909	1912	1915	rVV4	203821	339398	4.90%	0.760%
15	14.219	1915	1918	1924	rVB	542968	797263	11.52%	1.785%
16	14.390	1942	1947	1956	rVB	1748011	3066828	44.32%	6.865%
17	15.060	2059	2061	2065	rVB2	376514	415275	6.00%	0.930%
18	15.195	2079	2084	2088	rBV2	976720	1514764	21.89%	3.391%
19	15.907	2200	2205	2210	rBV	3142895	5033030	72.73%	11.267%
20	19.942	2888	2891	2897	rVB	5168982	6454104	93.27%	14.448%

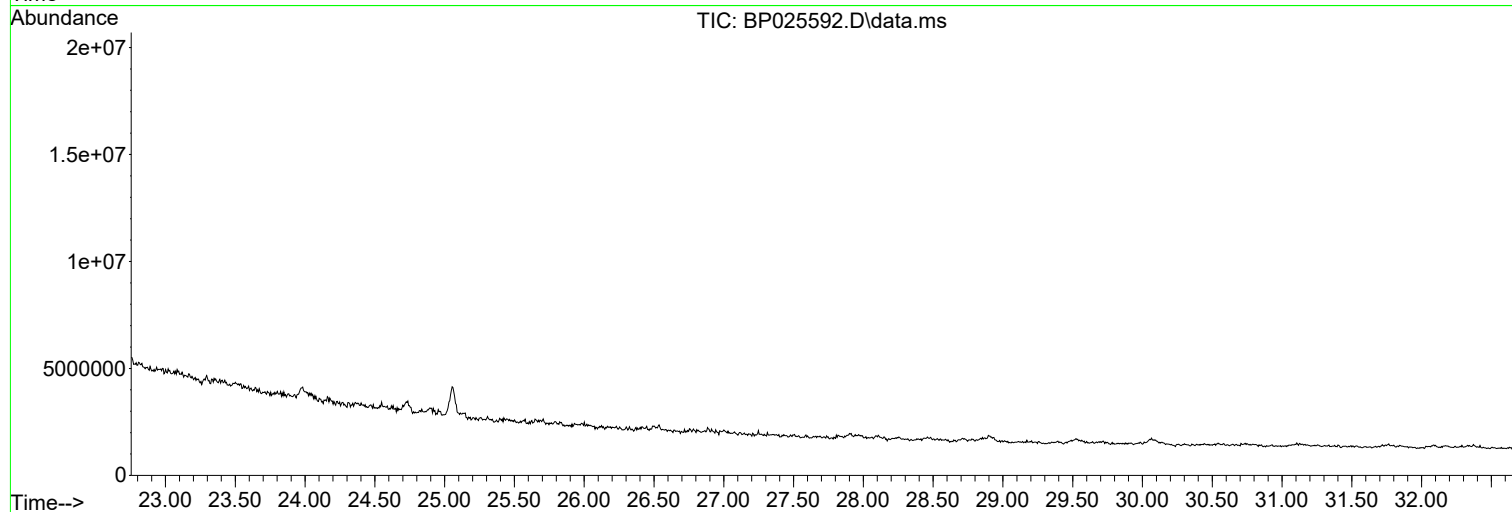
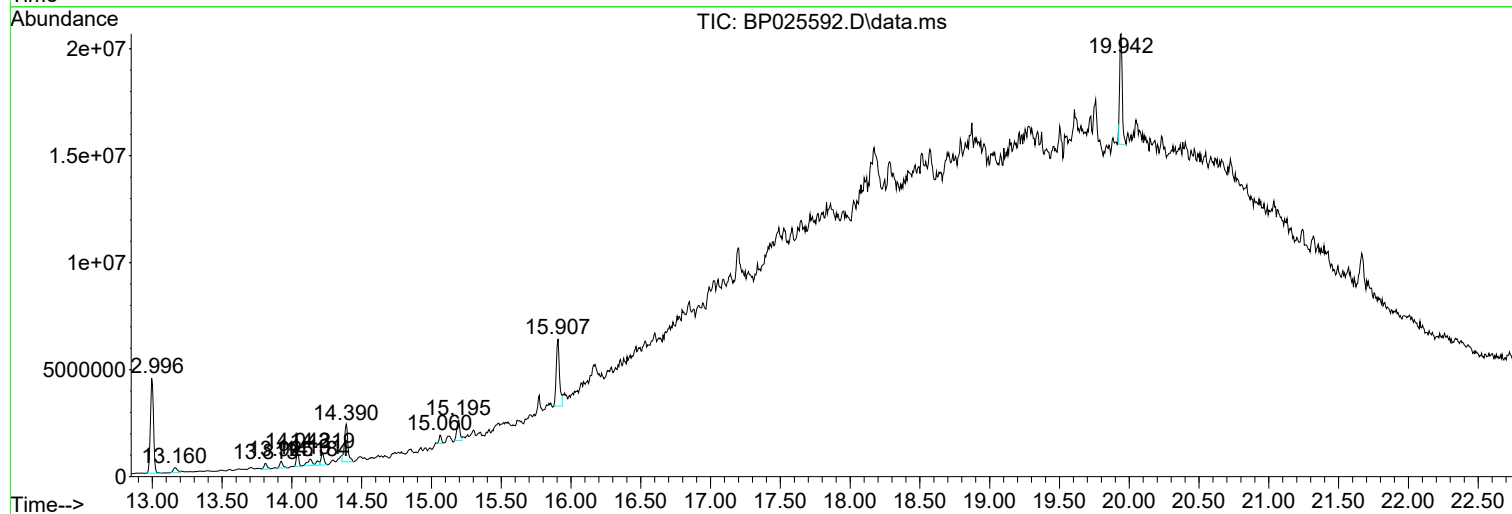
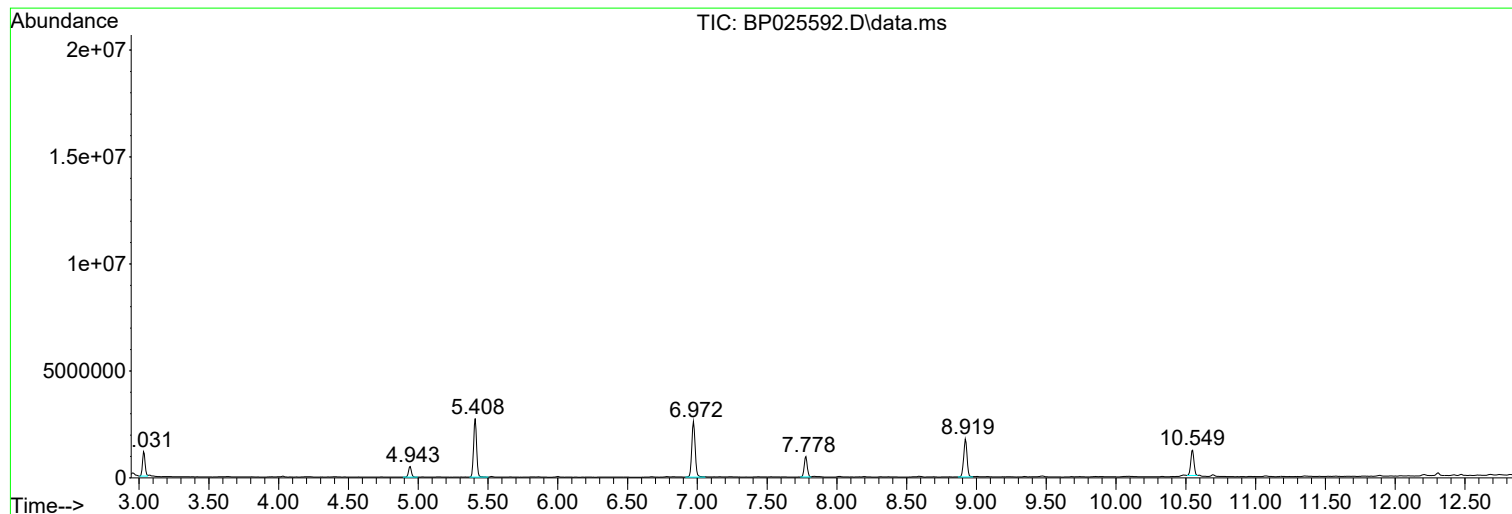
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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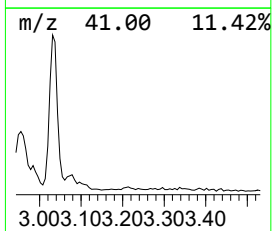
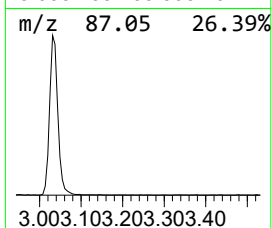
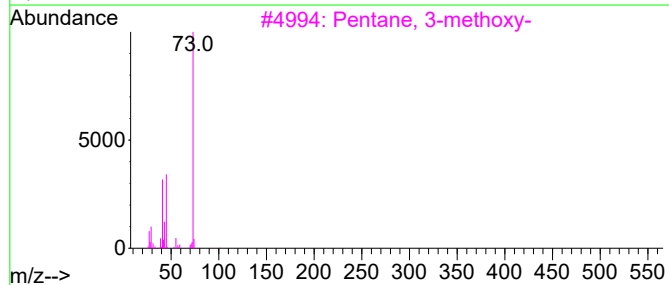
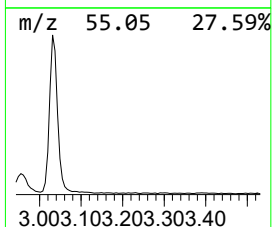
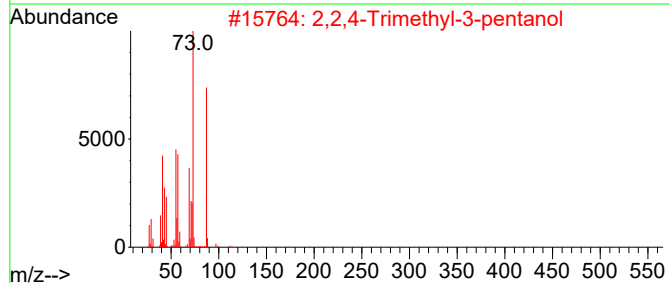
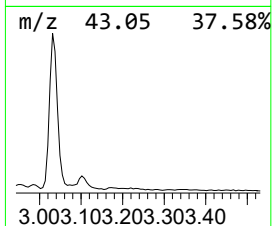
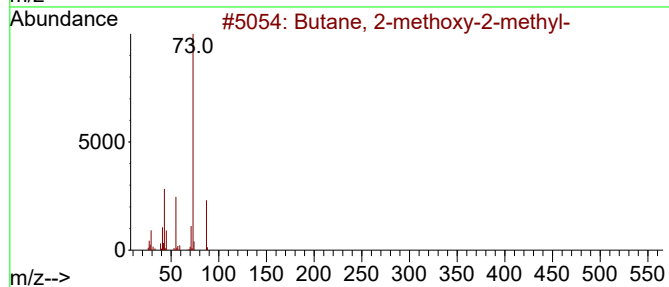
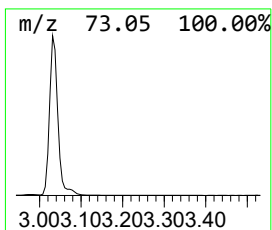
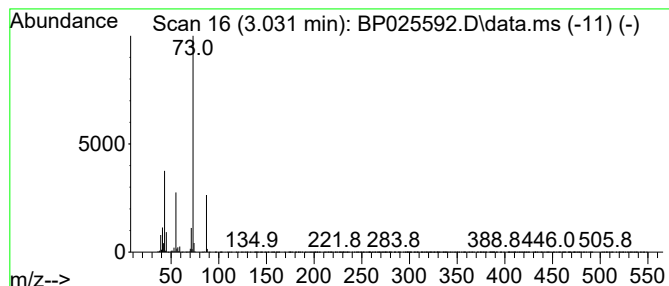
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.031	20.67 ng	1515340	1,4-Dichlorobenzene-d4	7.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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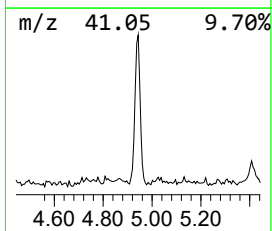
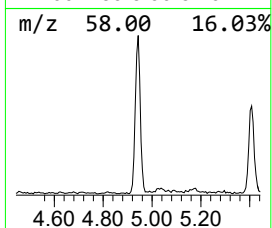
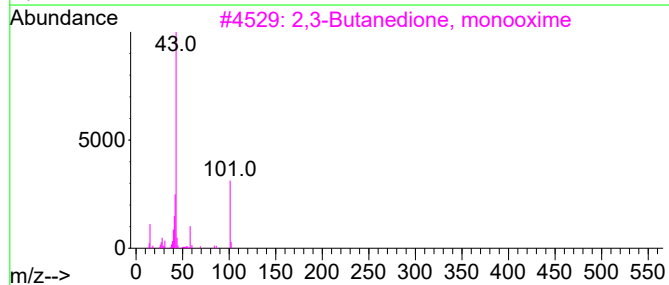
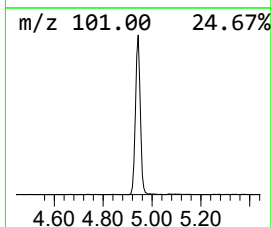
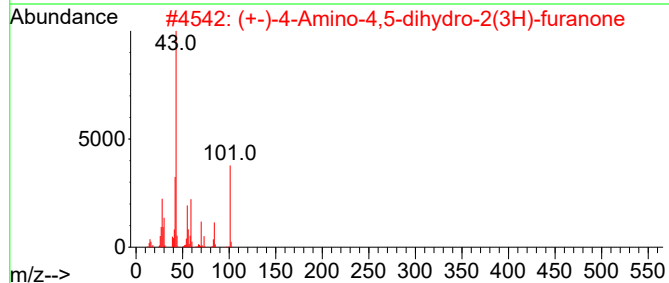
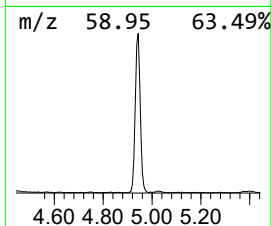
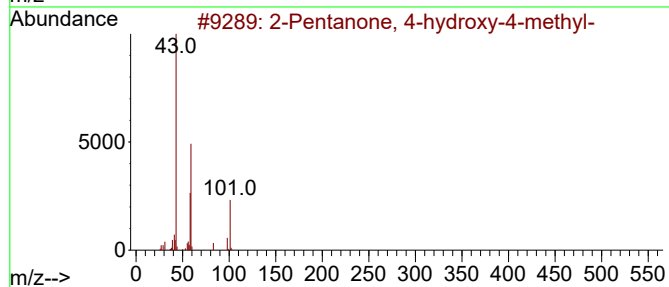
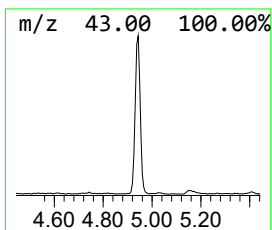
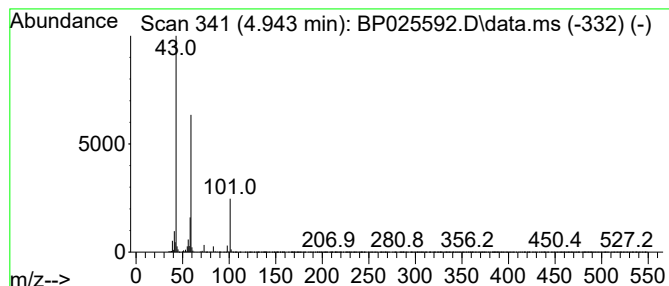
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.943	10.02 ng	734711	1,4-Dichlorobenzene-d4	7.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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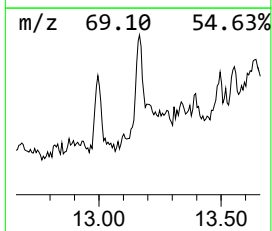
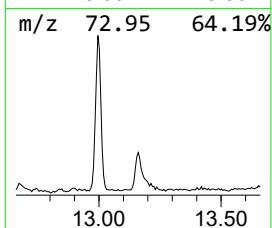
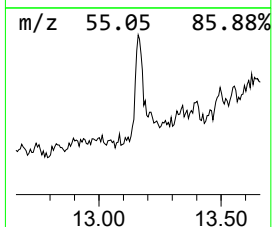
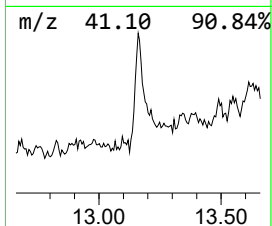
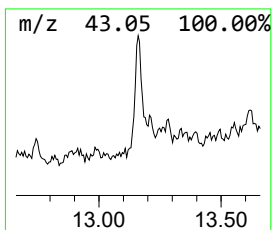
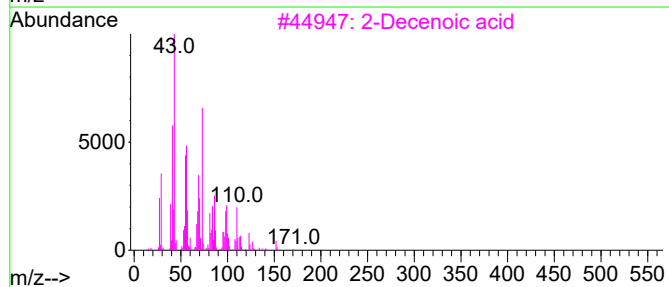
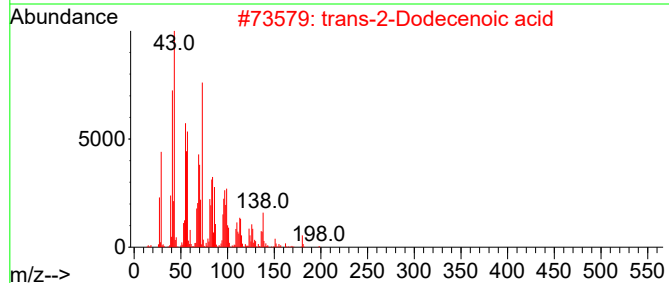
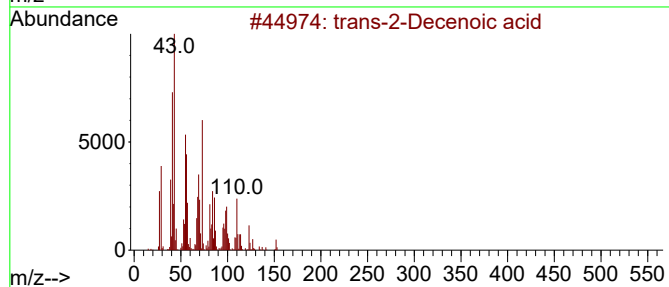
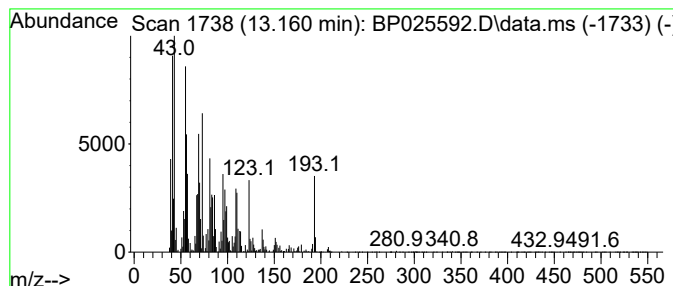
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 trans-2-Decenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.160	3.30 ng	506385	Acenaphthene-d10	14.390

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Decenoic acid	170	C10H18O2	000334-49-6	53
2			trans-2-Dodecenoic acid	198	C12H22O2	032466-54-9	43
3			2-Decenoic acid	170	C10H18O2	003913-85-7	41
4			trans-2-undecenoic acid	184	C11H20O2	015790-94-0	38
5			2-Tridecenoic acid, (E)-	212	C13H24O2	032466-55-0	38



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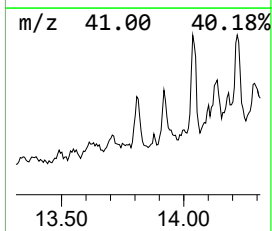
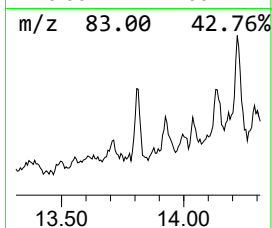
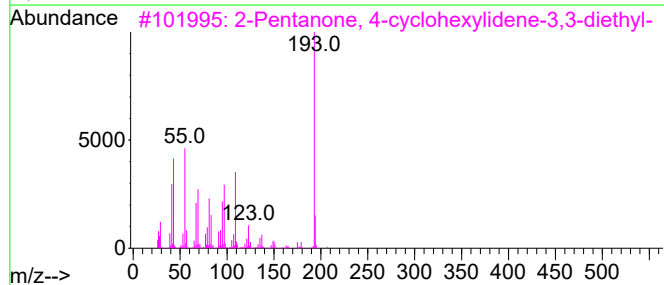
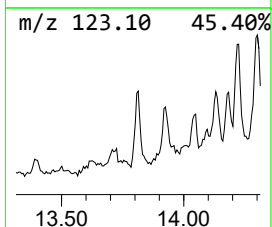
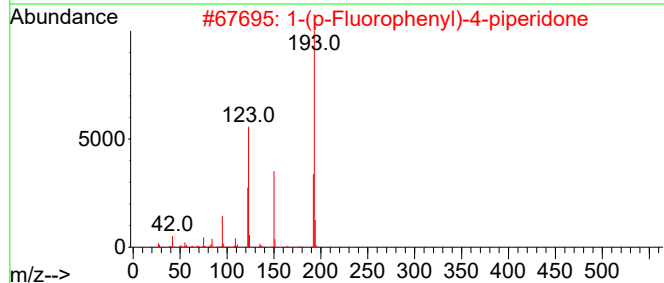
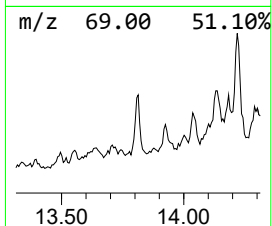
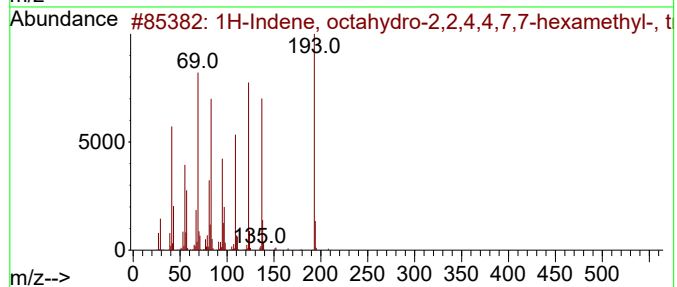
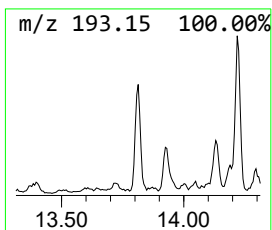
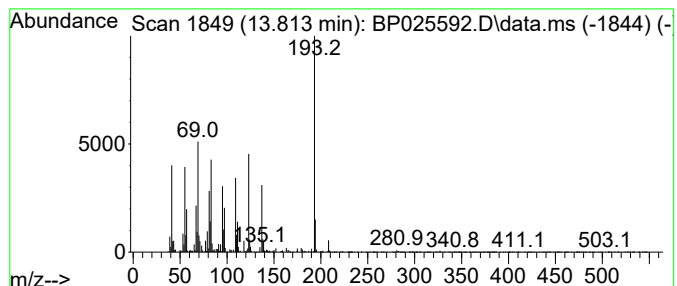
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1H-Indene, octahydro-2,2,4,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.813	2.87 ng	440154	Acenaphthene-d10	14.390

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	50
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	46
3			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	46
4			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
5			3H-3,10a-Methano-1,2-benzodioxoc...	226	C13H22O3	095906-83-5	38



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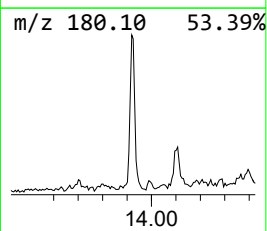
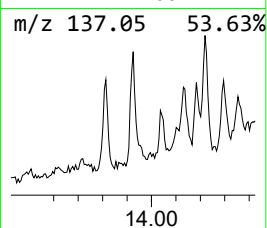
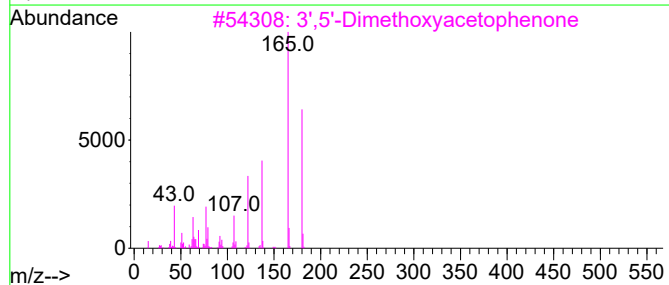
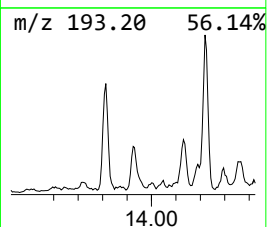
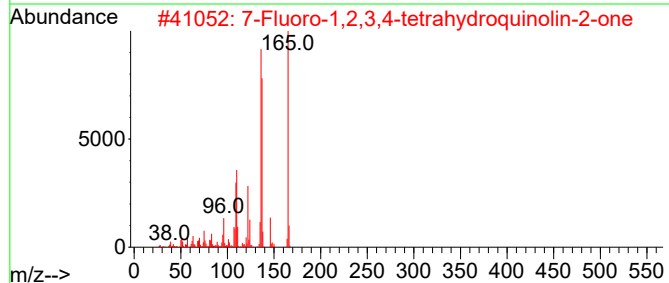
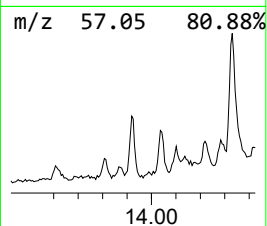
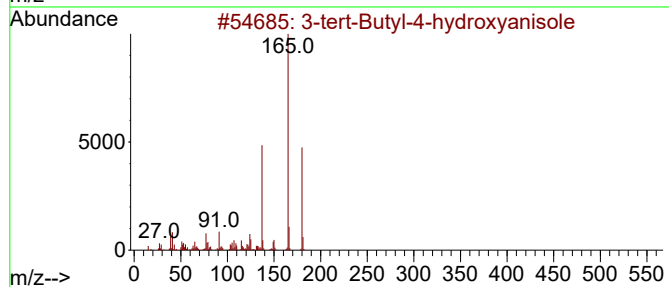
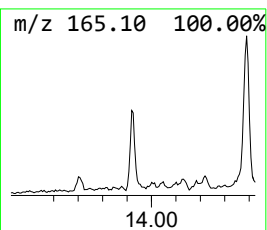
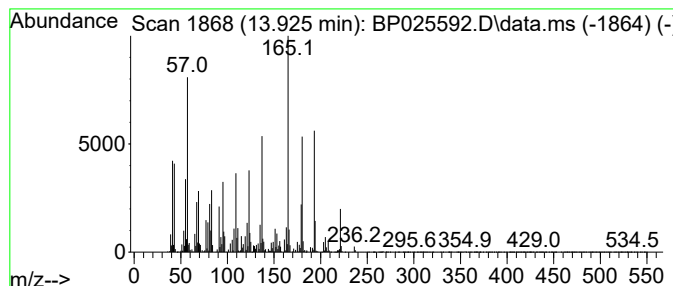
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-tert-Butyl-4-hydroxyanisole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.925	3.23 ng	495798	Acenaphthene-d10	14.390	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	50
2	7-Fluoro-1,2,3,4-tetrahydroquino...	165	C9H8FNO	004590-52-7	46
3	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	41
4	3-Methoxy-2-methyl-2H-pyrazolo[4...	165	C6H7N5O	037531-53-6	38
5	1,2,4-Cyclopentanetrione, 3-(2-p...	180	C10H12O3	054644-27-8	38



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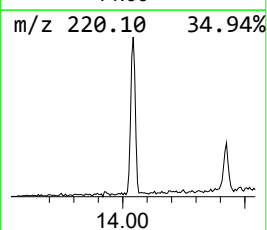
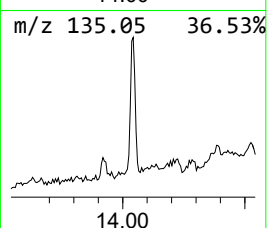
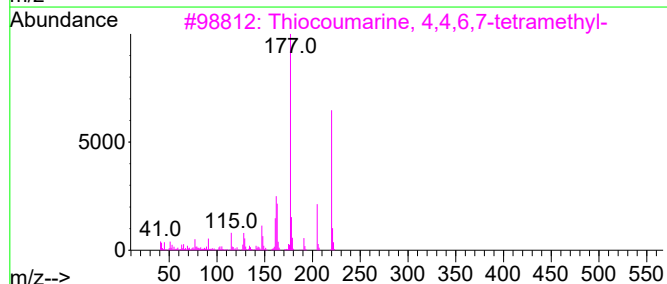
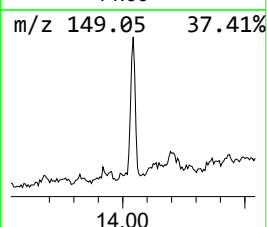
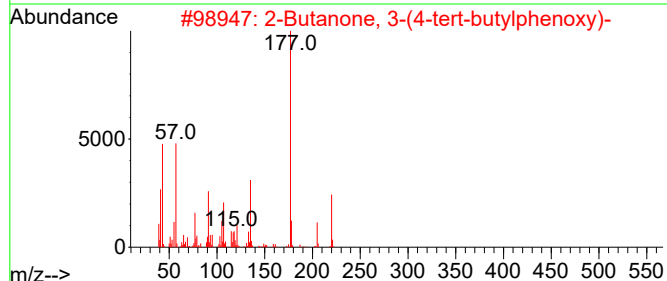
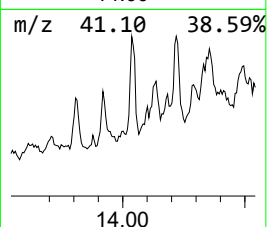
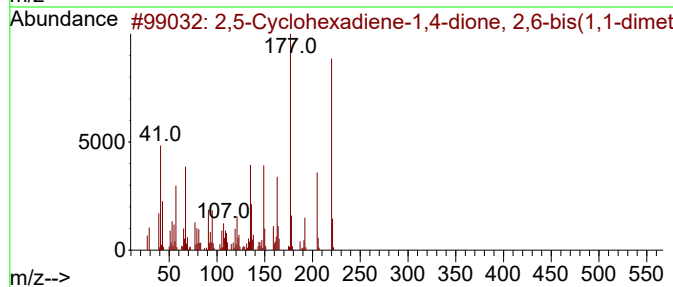
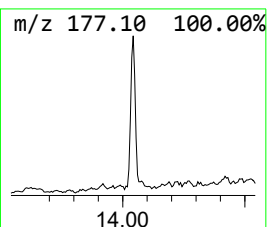
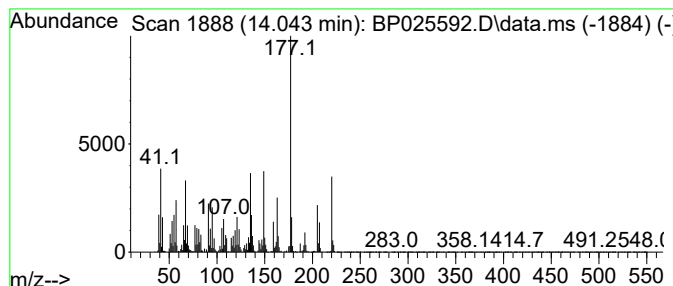
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.043	5.40 ng	828238	Acenaphthene-d10	14.390

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2		2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	60
3		Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	58
4		3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	46
5		2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082625\
Data File : BP025592.D
Acq On : 26 Aug 2025 19:22
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

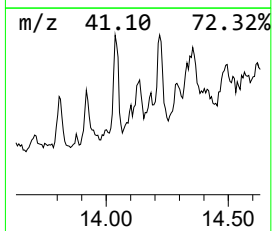
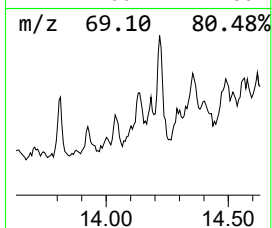
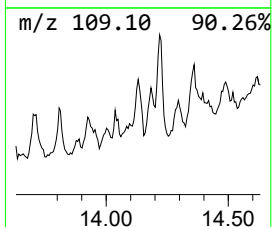
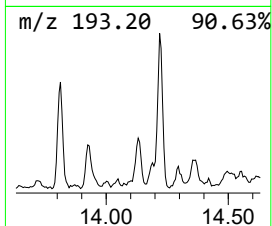
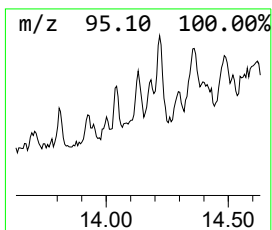
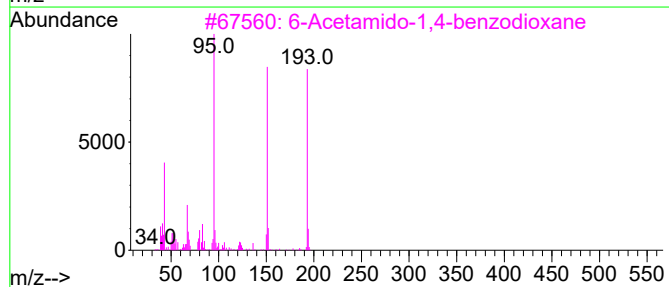
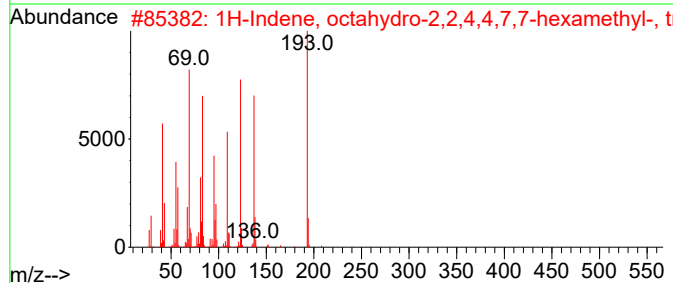
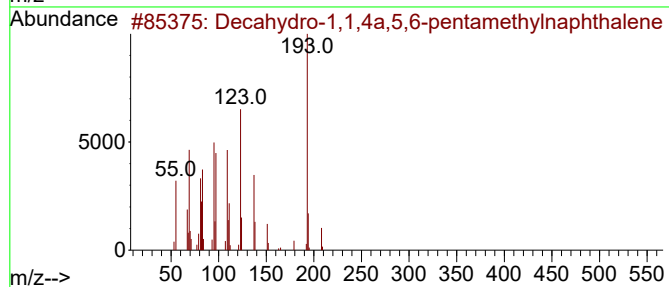
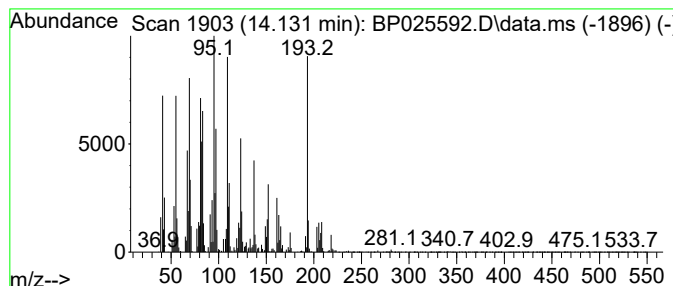
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.131	4.60 ng	705381	Acenaphthene-d10	14.390	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	53
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	30
4	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	25
5	Neopentylidenecyclohexane	152	C11H20	039546-80-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082625\
Data File : BP025592.D
Acq On : 26 Aug 2025 19:22
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

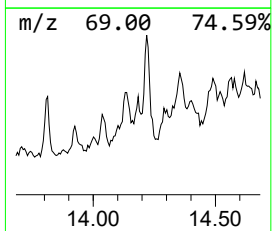
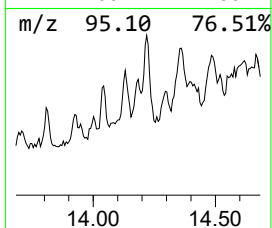
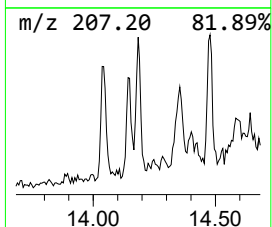
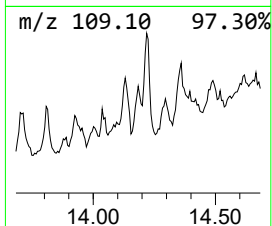
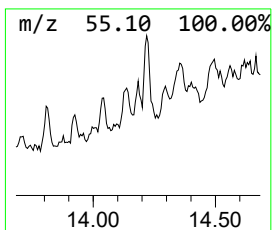
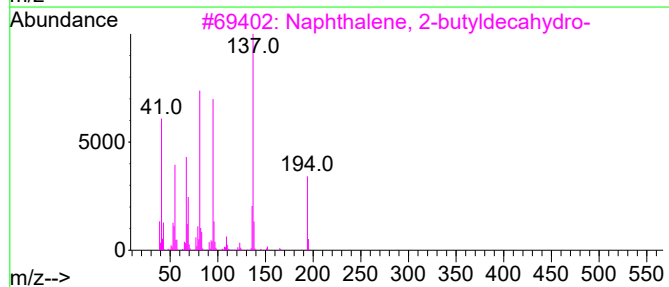
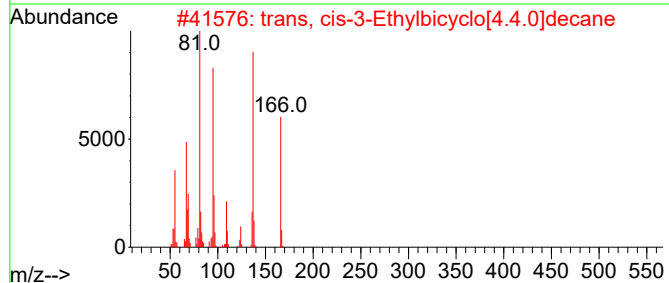
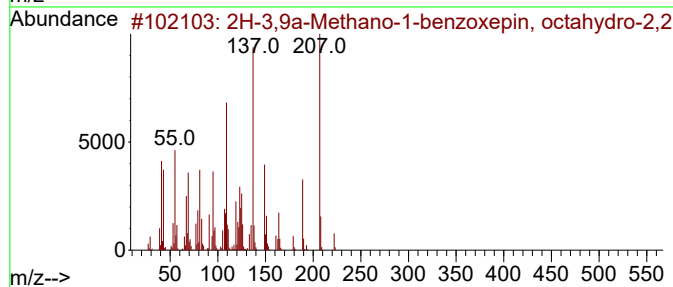
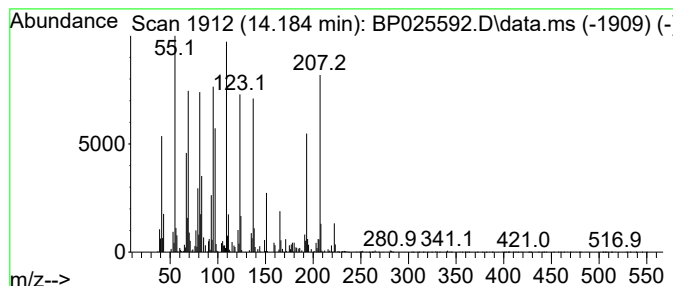
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2H-3,9a-Methano-1-benzoxepi... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.184	2.21 ng	339398	Acenaphthene-d10	14.390	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-3,9a-Methano-1-benzoxepin, oc...	222	C15H26O	005956-09-2	55
2	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	42
3	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	38
4	cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	30
5	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082625\
Data File : BP025592.D
Acq On : 26 Aug 2025 19:22
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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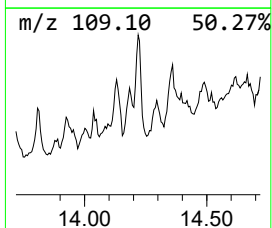
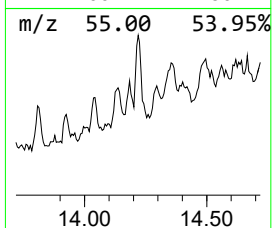
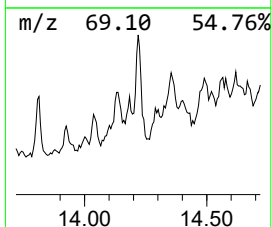
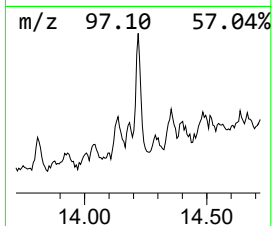
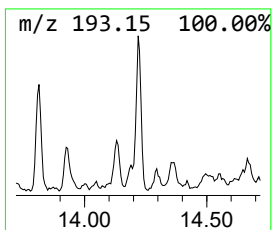
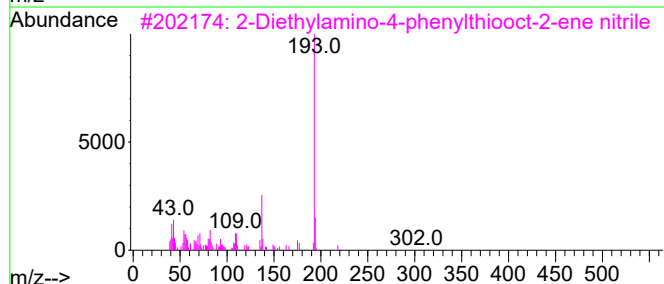
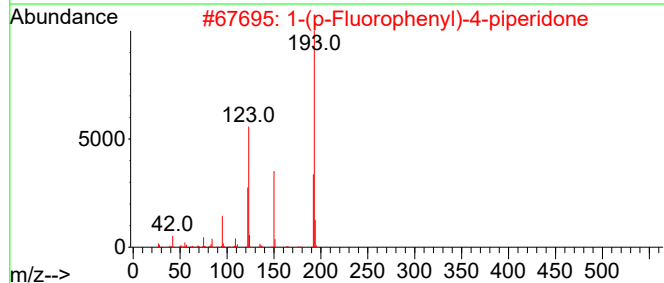
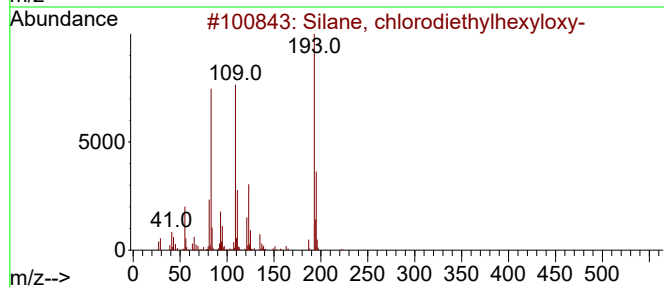
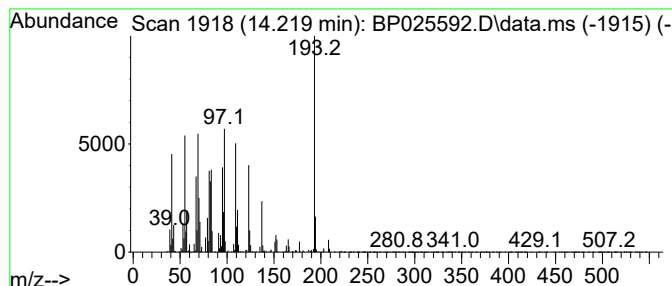
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.219 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	5.20 ng	797263	Acenaphthene-d10	14.390

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	35
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
3			2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	22
4			Acridine, 9-methyl-	193	C14H11N	000611-64-3	22
5			2-Phenylindolizine	193	C14H11N	025379-20-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082625\
Data File : BP025592.D
Acq On : 26 Aug 2025 19:22
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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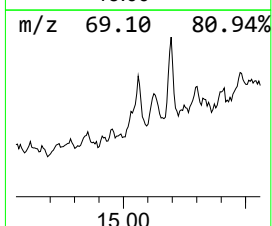
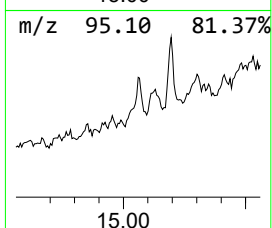
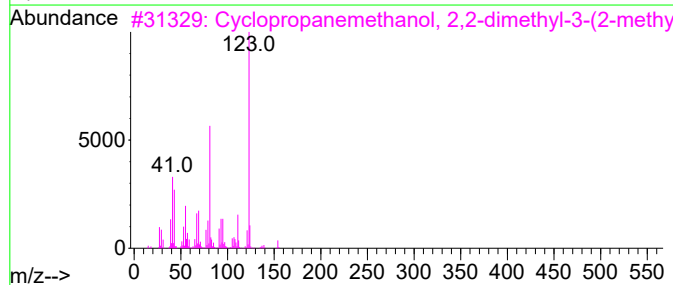
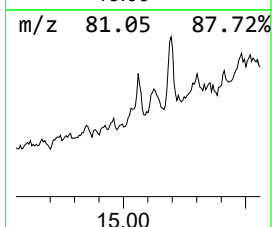
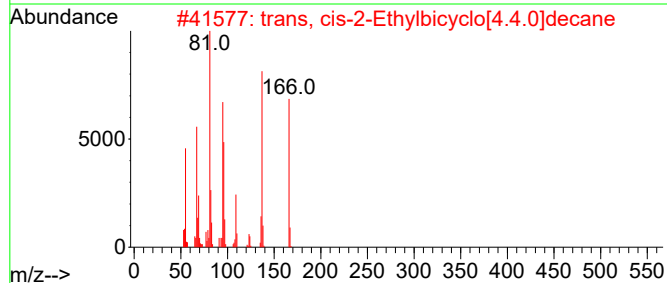
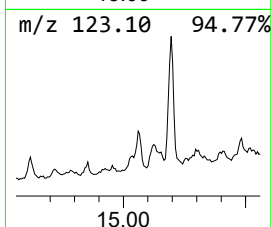
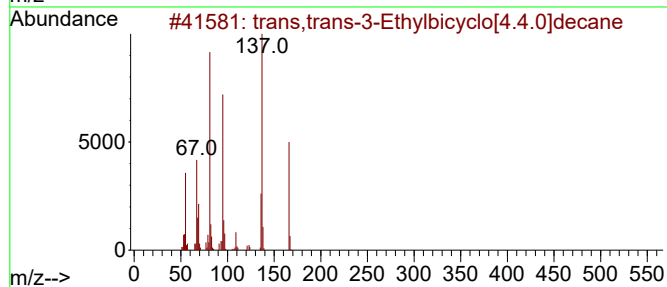
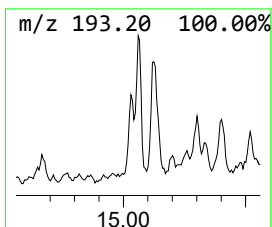
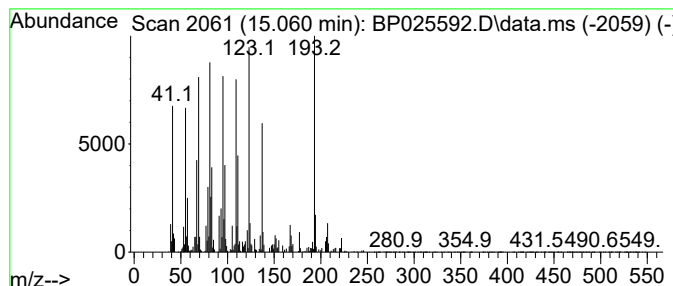
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.060 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.060	2.71 ng	415275	Acenaphthene-d10	14.390

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans,trans-3-Ethylbicyclo[4.4.0]...	166	C12H22	058462-32-1	30
2			trans, cis-2-Ethylbicyclo[4.4.0]...	166	C12H22	066660-39-7	25
3			Cyclopropanemethanol, 2,2-dimeth...	154	C10H18O	005617-92-5	20
4			cis-Chrysanthemyl alcohol	154	C10H18O	018383-59-0	18
5			Bicyclo[6.1.0]nonane, 9-bromo-9-...	216	C10H17Br	059474-03-2	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082625\
Data File : BP025592.D
Acq On : 26 Aug 2025 19:22
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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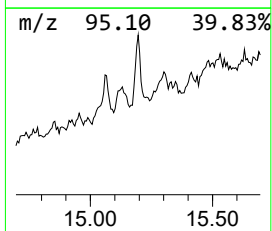
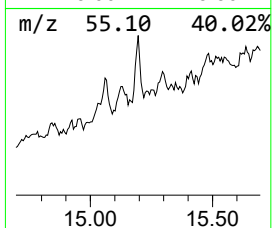
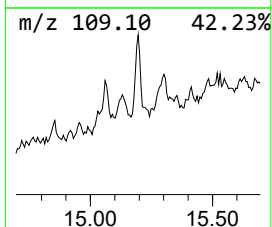
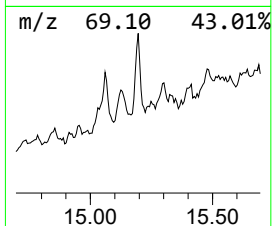
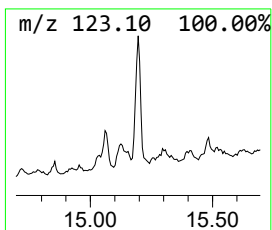
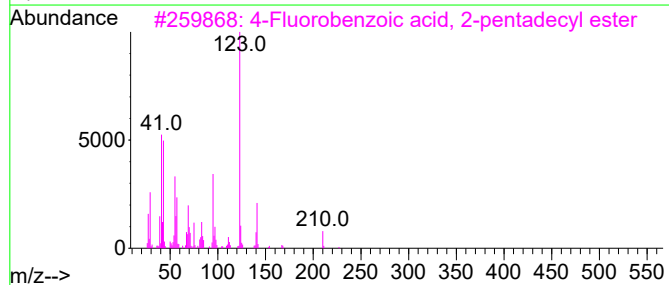
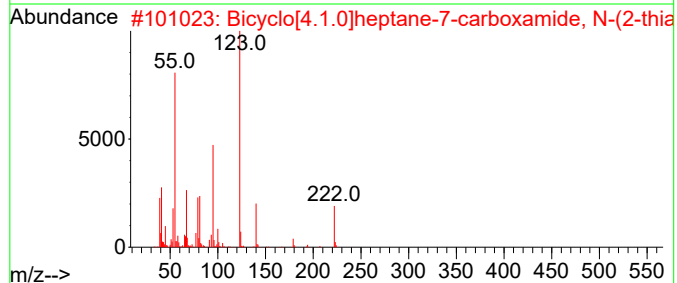
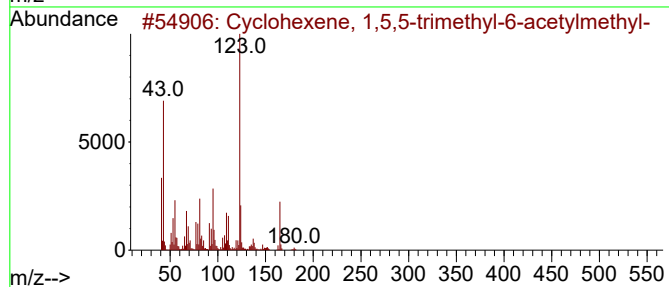
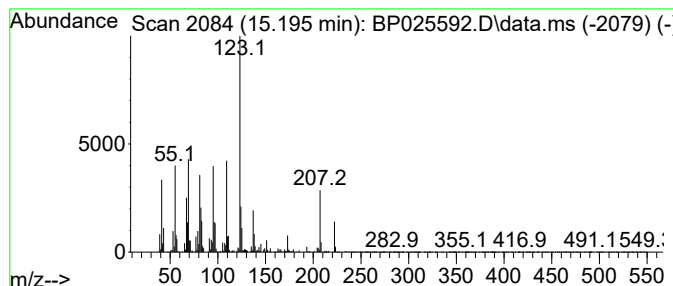
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclohexene, 1,5,5-trimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.195	9.88 ng	1514760	Acenaphthene-d10	14.390

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	53
2			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	38
3			4-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-68-3	38
4			1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	38
5			2-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000278-98-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082625\
Data File : BP025592.D
Acq On : 26 Aug 2025 19:22
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.031	20.7	ng	1515340	1	7.778	1466100	20.0
2-Pentanone, 4-...	4.943	10.0	ng	734711	1	7.778	1466100	20.0
trans-2-Decenoi...	13.160	3.3	ng	506385	3	14.390	3066830	20.0
1H-Indene, octa...	13.813	2.9	ng	440154	3	14.390	3066830	20.0
3-tert-Butyl-4-...	13.925	3.2	ng	495798	3	14.390	3066830	20.0
2,5-Cyclohexadi...	14.043	5.4	ng	828238	3	14.390	3066830	20.0
Decahydro-1,1,4...	14.131	4.6	ng	705381	3	14.390	3066830	20.0
2H-3,9a-Methano...	14.184	2.2	ng	339398	3	14.390	3066830	20.0
unknown14.219	14.219	5.2	ng	797263	3	14.390	3066830	20.0
unknown15.060	15.060	2.7	ng	415275	3	14.390	3066830	20.0
Cyclohexene, 1,...	15.195	9.9	ng	1514760	3	14.390	3066830	20.0