

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080825\
 Data File : BP025333.D
 Acq On : 08 Aug 2025 15:11
 Operator : CG/JU
 Sample : Q2795-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-1

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: BP025333.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	14	rVB2	261902	405233	3.84%	0.561%
2	3.043	14	18	32	rVB	1799577	2267043	21.48%	3.137%
3	4.355	236	241	249	rBV	361097	474511	4.50%	0.657%
4	4.949	334	342	351	rBV	512854	721193	6.83%	0.998%
5	5.408	410	420	428	rBV	3499729	5153505	48.83%	7.132%
6	6.966	675	685	693	rBV	3371977	5214879	49.41%	7.217%
7	7.796	819	826	833	rBV	1288545	2133856	20.22%	2.953%
8	8.937	1012	1020	1031	rVB	2139006	3679447	34.86%	5.092%
9	10.572	1290	1298	1310	rVB	1782968	2987972	28.31%	4.135%
10	13.037	1709	1717	1724	rBV	5227139	8035781	76.14%	11.120%
11	14.425	1946	1953	1959	rBV	2556179	3818462	36.18%	5.284%
12	15.801	2181	2187	2195	rVB	856622	1106095	10.48%	1.531%
13	15.925	2201	2208	2218	rBV	3738617	6211061	58.85%	8.595%
14	17.225	2423	2429	2434	rBV	3166977	4465151	42.31%	6.179%
15	17.266	2434	2436	2442	rVB	228055	258372	2.45%	0.358%
16	18.178	2586	2591	2603	rBV	1998249	2809345	26.62%	3.888%
17	19.348	2785	2790	2799	rBV	467732	682325	6.46%	0.944%
18	19.501	2811	2816	2828	rBV	706368	1076882	10.20%	1.490%
19	19.719	2846	2853	2857	rBV	394445	598327	5.67%	0.828%
20	19.954	2887	2893	2903	rVB	8525701	10554302	100.00%	14.605%
21	21.348	3126	3130	3141	rVB2	754391	1137473	10.78%	1.574%
22	21.660	3176	3183	3190	rBV2	1995407	3896334	36.92%	5.392%
23	21.830	3209	3212	3218	rVB	129496	189028	1.79%	0.262%
24	23.313	3459	3464	3474	rBV	429670	944363	8.95%	1.307%
25	25.054	3752	3760	3775	rVB	1216888	3441788	32.61%	4.763%

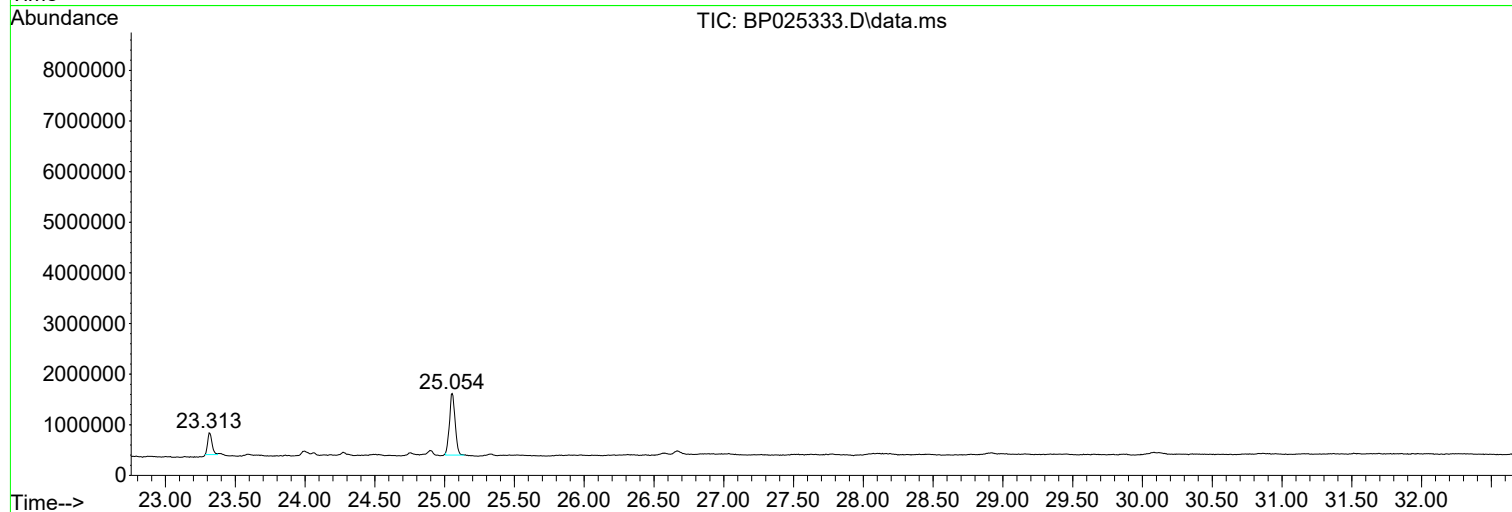
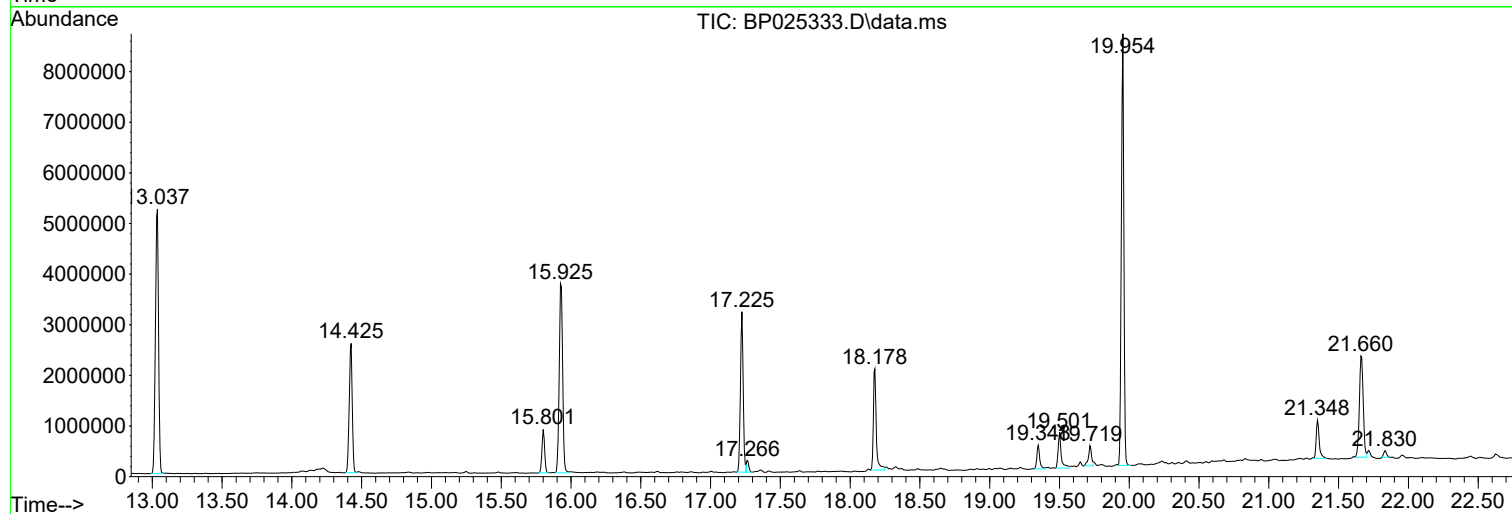
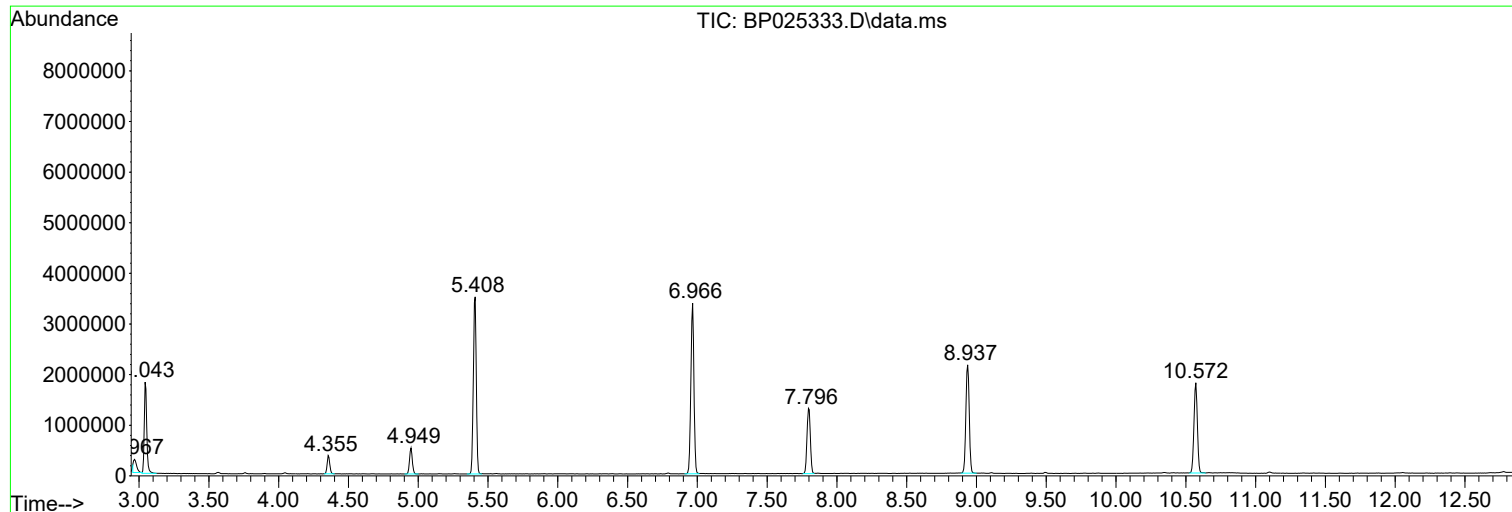
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BP025333.D
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Instrument :
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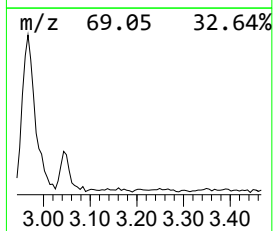
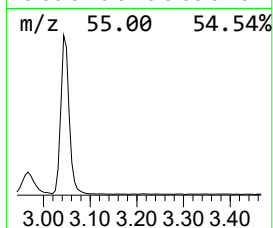
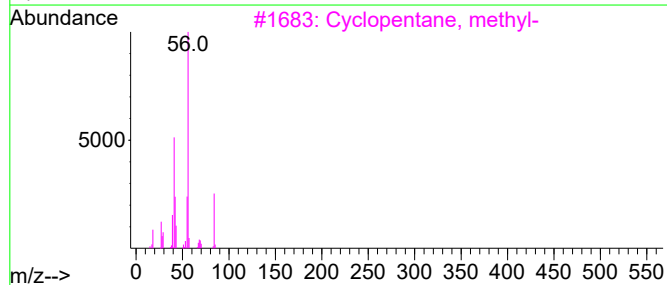
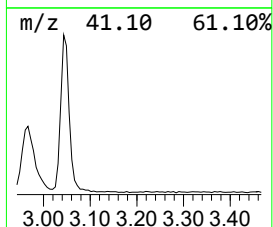
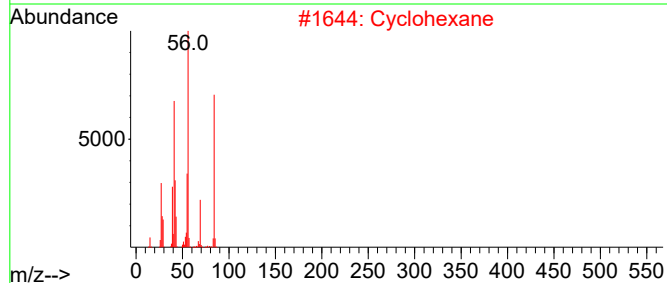
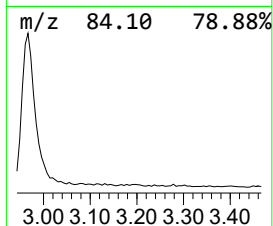
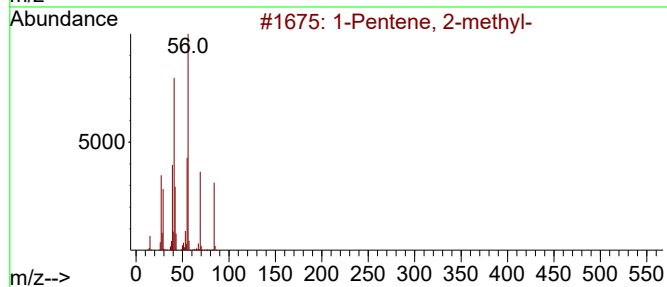
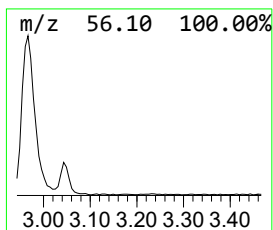
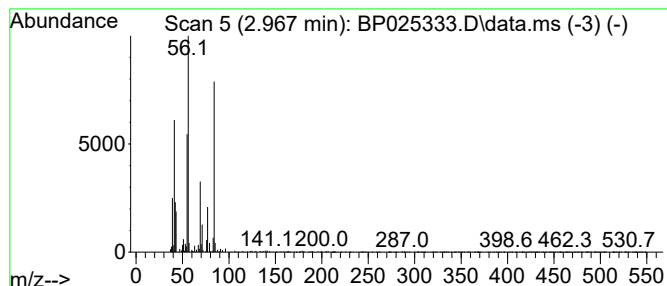
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.967	3.80 ng	405233	1,4-Dichlorobenzene-d4	7.802

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
2			Cyclohexane	84	C6H12	000110-82-7	72
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	64
4			Pyridine-D5-	84	C5D5N	007291-22-7	59
5			Cyclopentanone	84	C5H8O	000120-92-3	47



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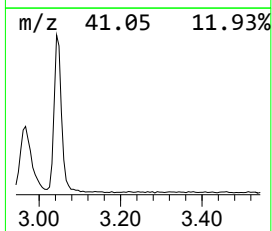
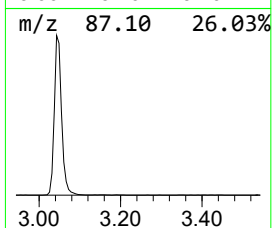
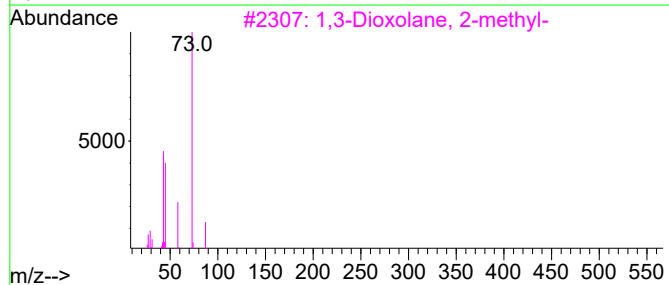
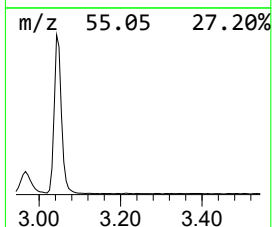
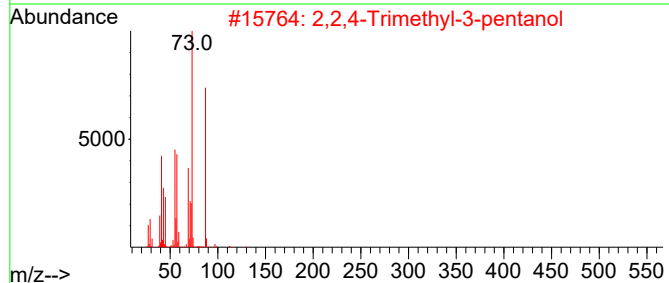
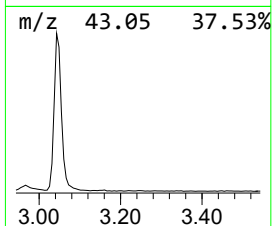
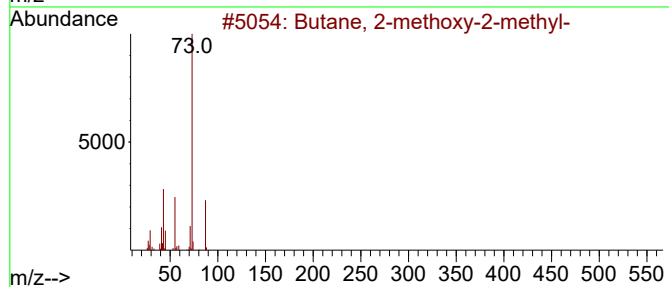
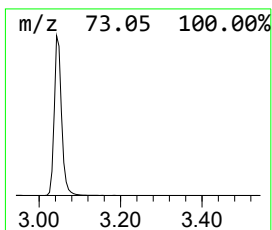
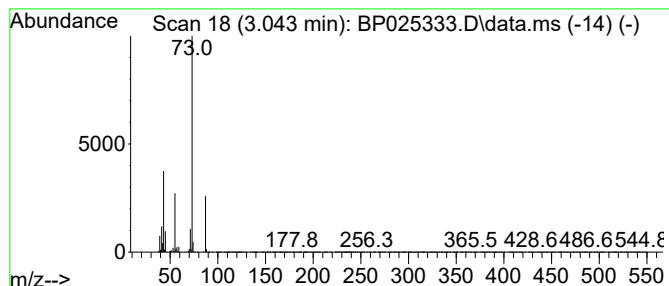
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.043	21.25 ng	2267040	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	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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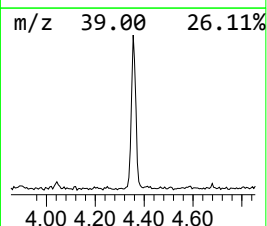
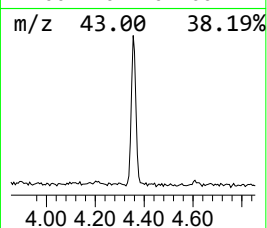
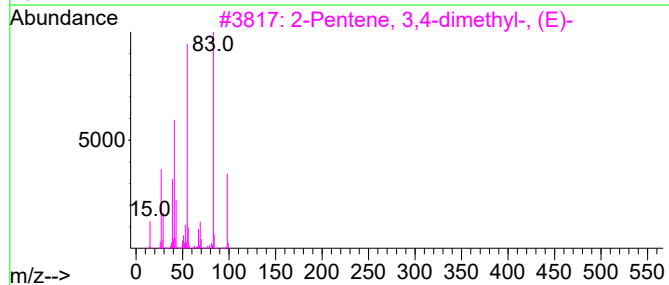
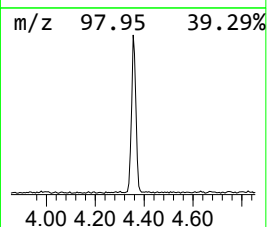
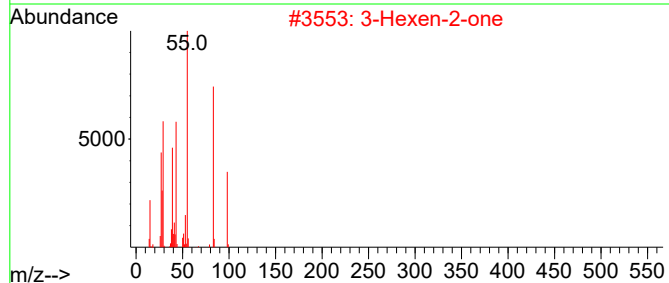
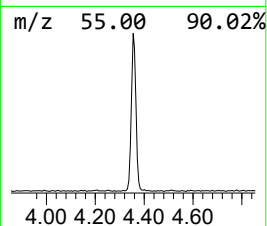
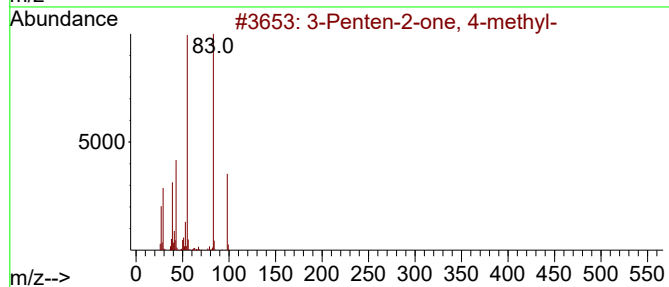
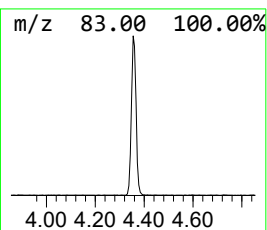
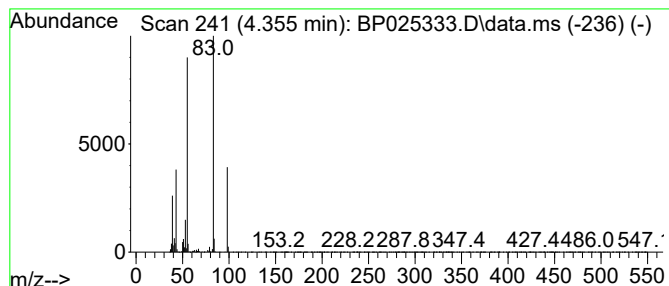
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.355	4.45 ng	474511	1,4-Dichlorobenzene-d4	7.802

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N02	042282-85-9	78



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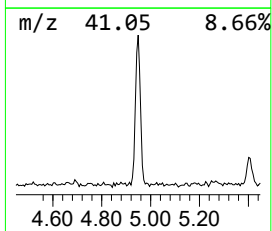
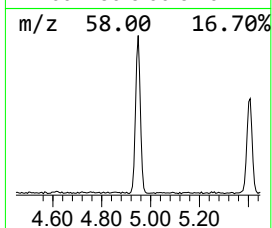
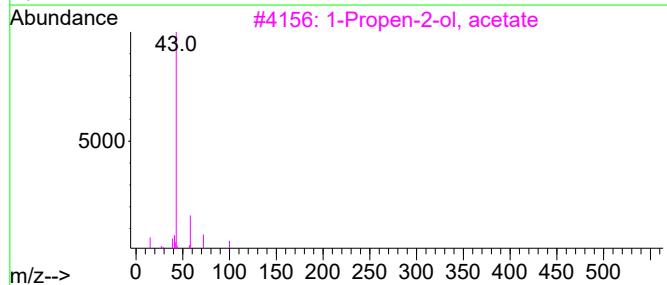
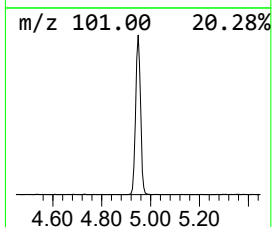
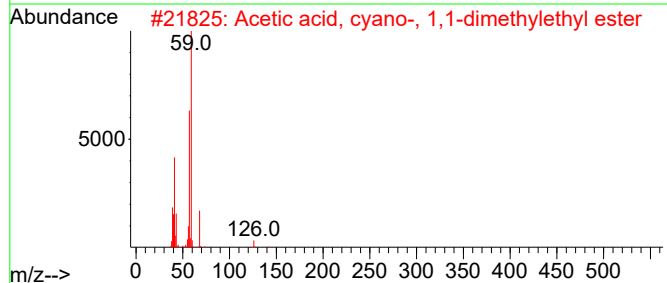
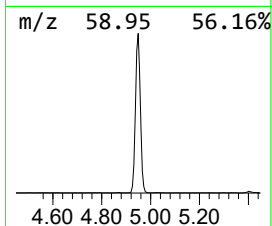
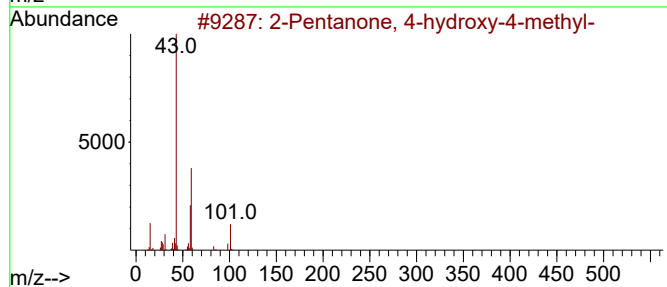
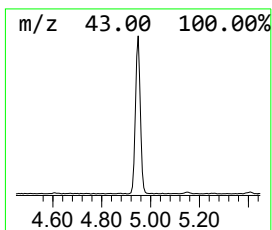
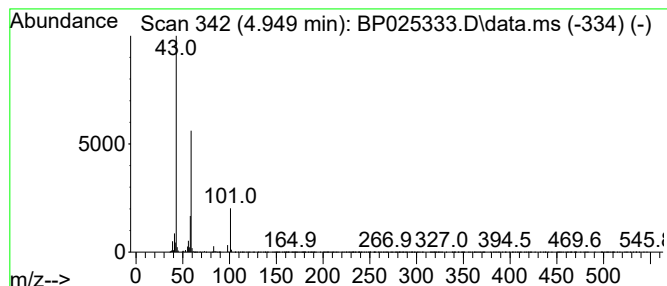
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.949	6.76 ng	721193	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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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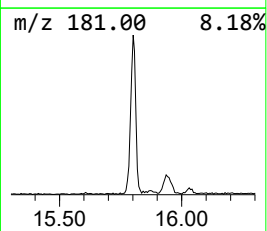
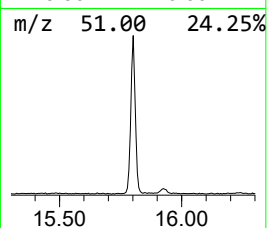
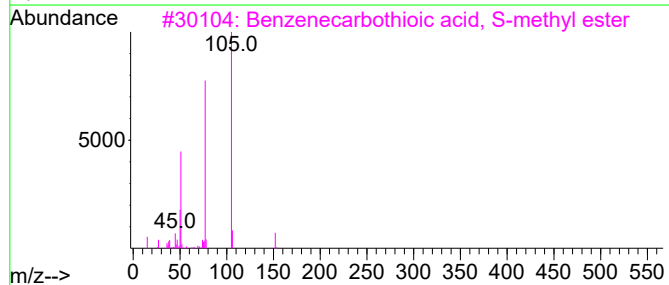
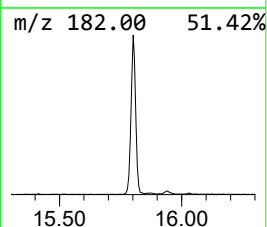
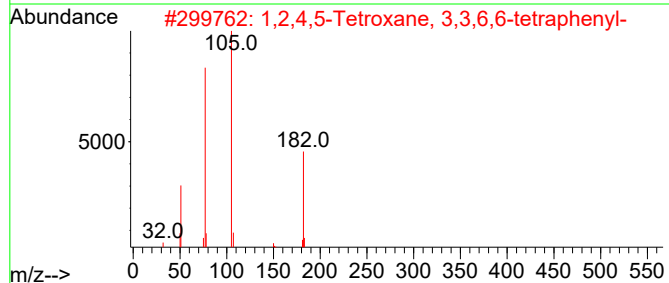
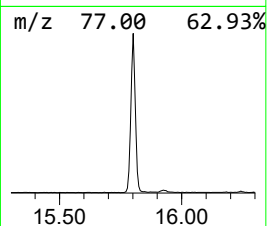
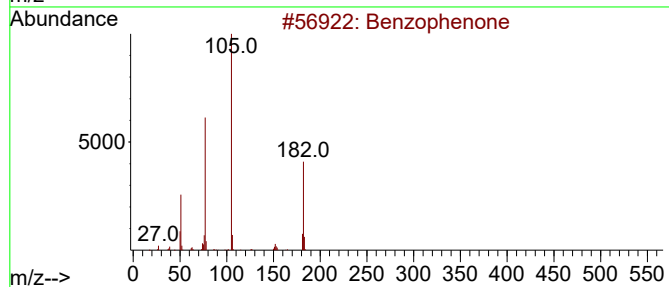
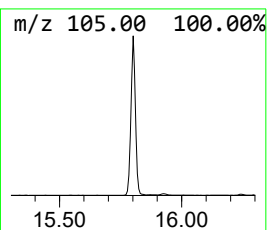
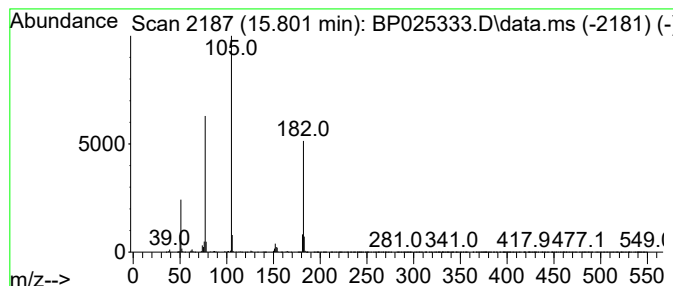
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.801	5.79 ng	1106100	Acenaphthene-d10	14.425

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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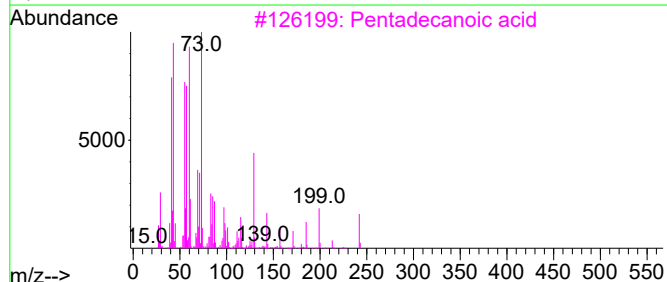
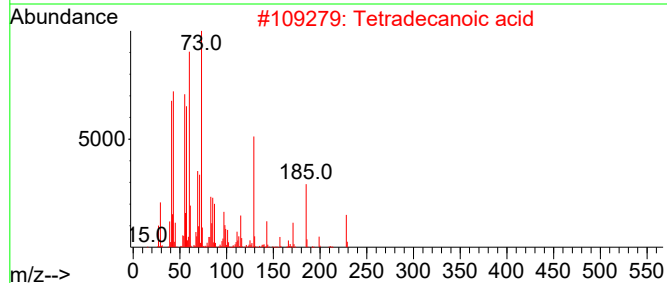
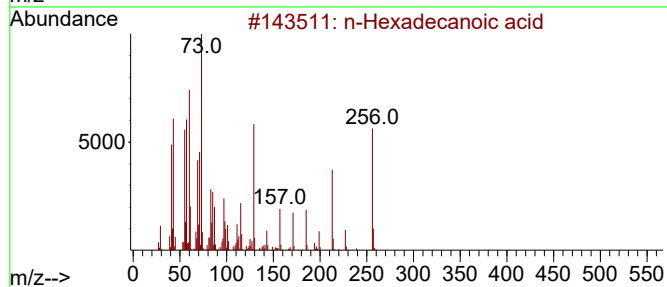
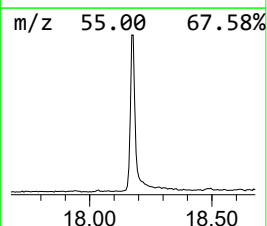
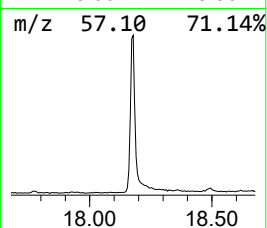
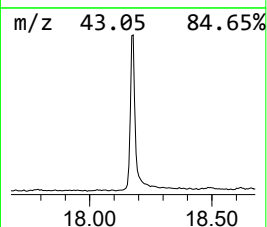
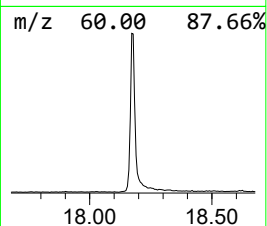
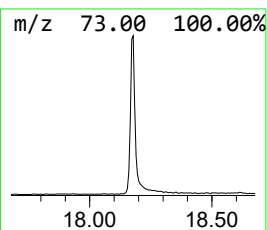
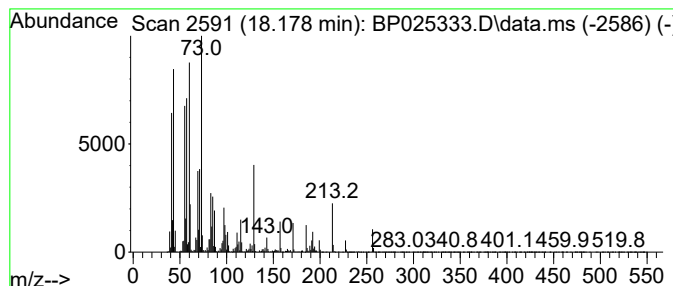
Instrument :
BNA_P
ClientSampleId :
COMP-1

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 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.177	12.58 ng	2809350	Phenanthrene-d10		17.225	
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	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
4	Tridecanoic acid		214	C13H26O2	000638-53-9	80
5	n-Decanoic acid		172	C10H20O2	000334-48-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080825\
Data File : BP025333.D
Acq On : 08 Aug 2025 15:11
Operator : CG/JU
Sample : Q2795-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

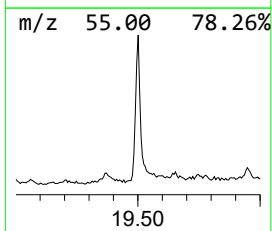
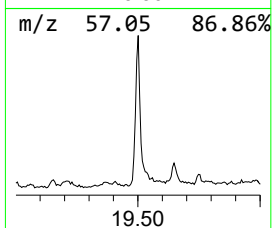
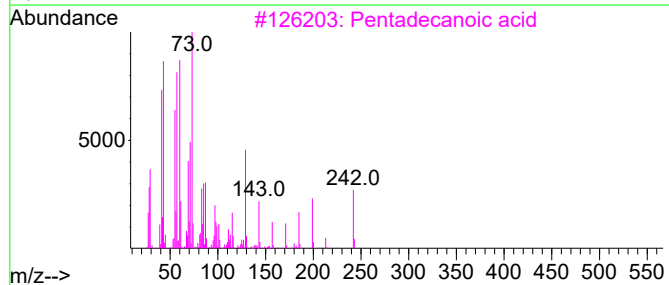
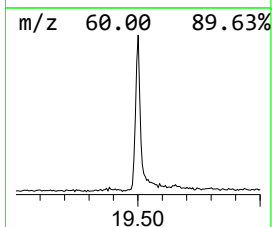
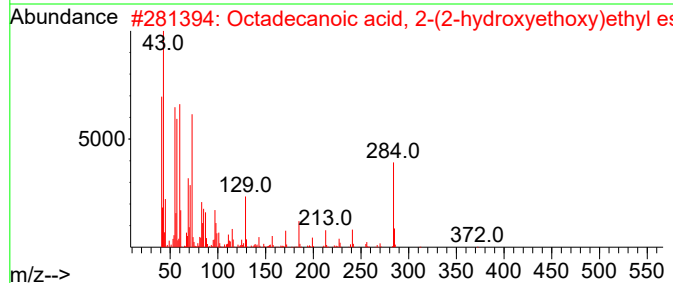
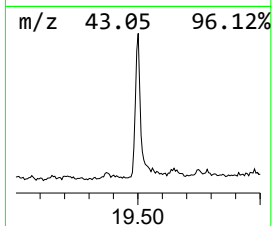
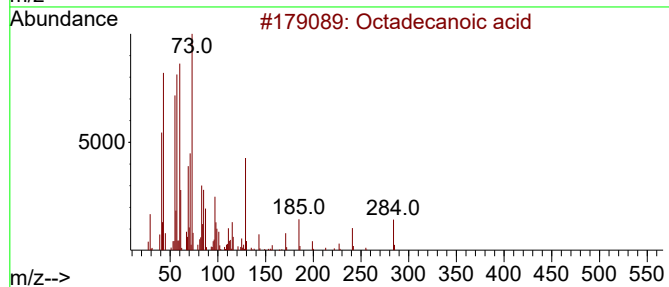
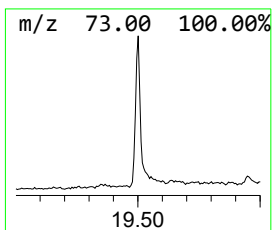
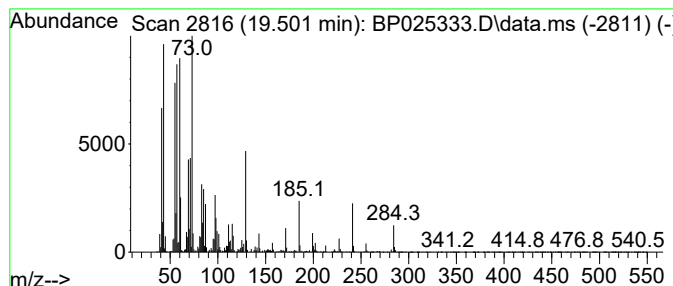
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.501	5.53 ng	1076880	Chrysene-d12	21.660

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080825\
Data File : BP025333.D
Acq On : 08 Aug 2025 15:11
Operator : CG/JU
Sample : Q2795-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

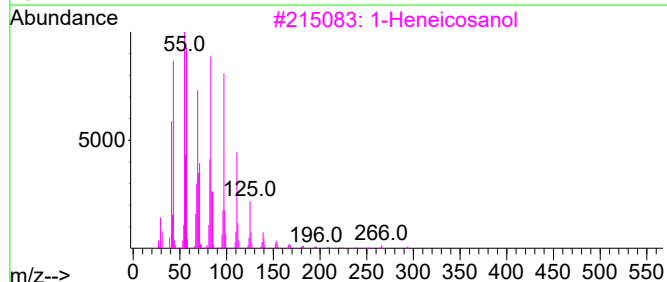
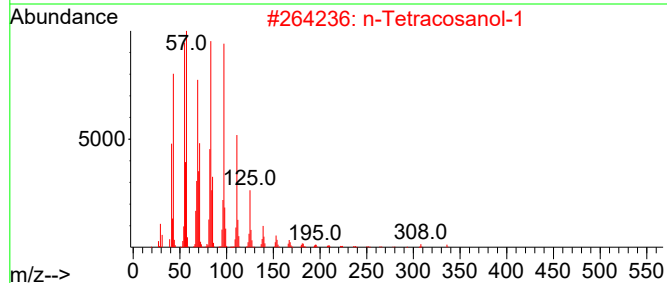
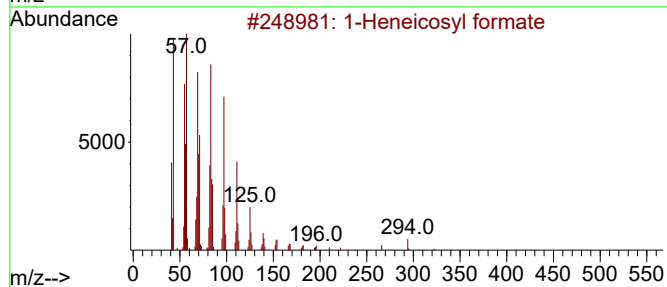
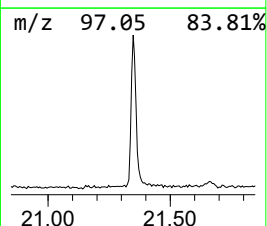
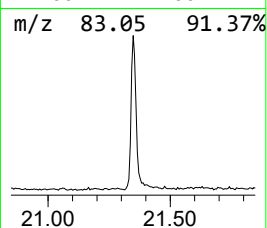
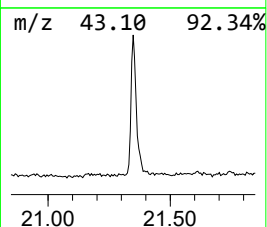
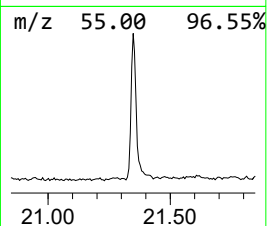
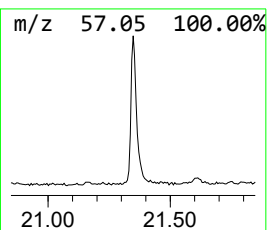
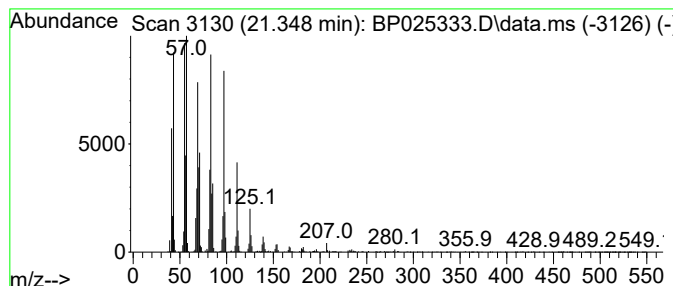
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.348	5.84 ng	1137470	Chrysene-d12	21.660	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	97
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	Pentacos-1-ene	350	C25H50	016980-85-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080825\
Data File : BP025333.D
Acq On : 08 Aug 2025 15:11
Operator : CG/JU
Sample : Q2795-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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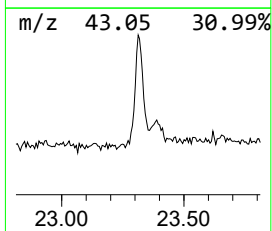
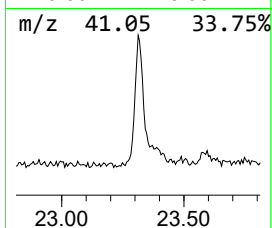
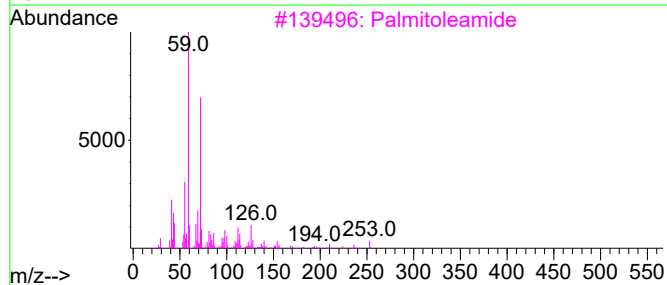
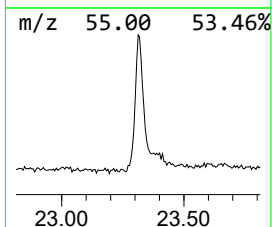
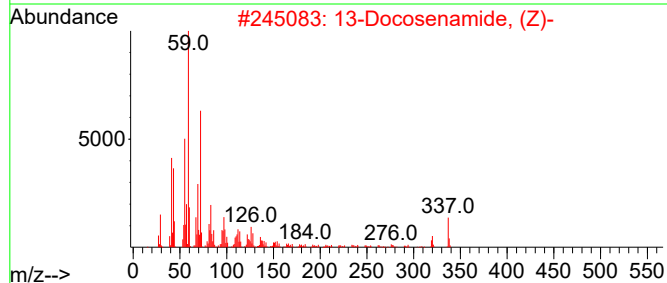
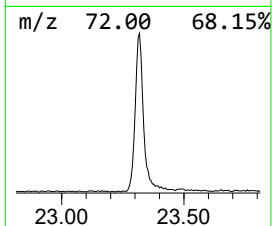
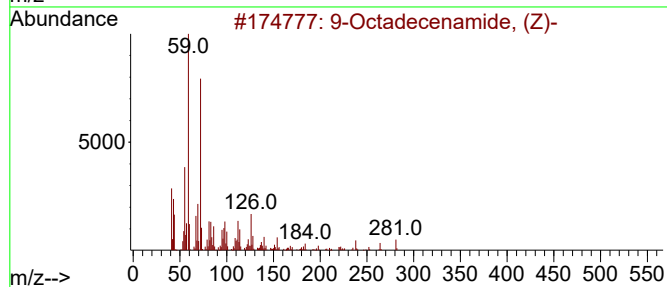
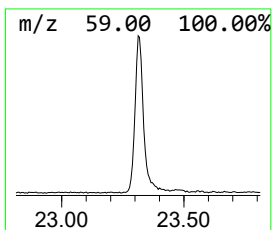
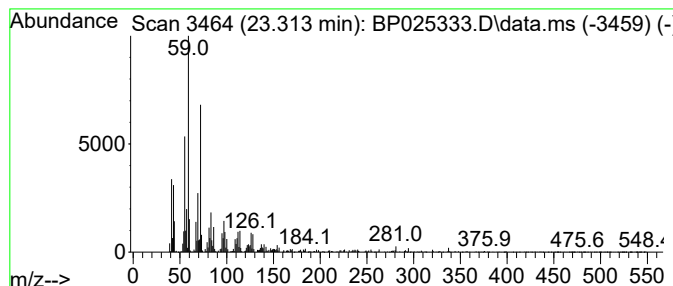
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.313	4.85 ng	944363	Chrysene-d12	21.660

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3			Palmitoleamide	253	C16H31NO	106010-22-4	86
4			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080825\
Data File : BP025333.D
Acq On : 08 Aug 2025 15:11
Operator : CG/JU
Sample : Q2795-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Pentene, 2-me...	2.967	3.8	ng	405233	1	7.802	2133860	20.0
Butane, 2-metho...	3.043	21.3	ng	2267040	1	7.802	2133860	20.0
3-Penten-2-one,...	4.355	4.5	ng	474511	1	7.802	2133860	20.0
2-Pentanone, 4-...	4.949	6.8	ng	721193	1	7.802	2133860	20.0
Benzophenone	15.801	5.8	ng	1106100	3	14.425	3818460	20.0
n-Hexadecanoic ...	18.177	12.6	ng	2809350	4	17.225	4465150	20.0
Octadecanoic acid	19.501	5.5	ng	1076880	5	21.660	3896330	20.0
1-Heneicosyl fo...	21.348	5.8	ng	1137470	5	21.660	3896330	20.0
9-Octadecenamid...	23.313	4.8	ng	944363	5	21.660	3896330	20.0