

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
 Data File : BP024815.D
 Acq On : 28 May 2025 14:49
 Operator : RC/JU
 Sample : Q2128-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP03-MHM

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-BP051325.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024815.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.816	288	294	303	rBV	104740	151761	2.89%	0.450%
2	5.275	366	372	385	rBV	1112442	1712704	32.67%	5.083%
3	6.846	632	639	659	rBV	1038288	1800256	34.34%	5.343%
4	7.646	769	775	784	rBV	300287	466782	8.90%	1.385%
5	8.793	963	970	987	rBV	570551	1058876	20.20%	3.143%
6	10.416	1236	1246	1252	rBV	361843	634667	12.11%	1.884%
7	12.881	1658	1665	1686	rBV	1466033	2277387	43.44%	6.759%
8	14.004	1849	1856	1861	rBV4	43708	109352	2.09%	0.325%
9	14.057	1861	1865	1869	rVV5	31570	58392	1.11%	0.173%
10	14.187	1873	1887	1891	rVV	409261	979635	18.69%	2.908%
11	14.251	1893	1898	1899	rVV	548783	868406	16.56%	2.577%
12	14.275	1899	1902	1909	rVB	727965	1176728	22.45%	3.493%
13	14.716	1975	1977	1989	rVB4	40262	91245	1.74%	0.271%
14	15.657	2132	2137	2149	rBV	212587	366766	7.00%	1.089%
15	15.798	2154	2161	2176	rBV	1669226	2799334	53.40%	8.309%
16	16.492	2273	2279	2292	rBV7	50596	136867	2.61%	0.406%
17	17.069	2372	2377	2382	rBV	766299	1059266	20.20%	3.144%
18	17.116	2382	2385	2392	rVB	176408	247506	4.72%	0.735%
19	17.210	2397	2401	2407	rVV	45784	77841	1.48%	0.231%
20	17.286	2408	2414	2420	rVB2	46422	89987	1.72%	0.267%
21	18.010	2531	2537	2546	rBV	1149389	1763334	33.63%	5.234%
22	18.175	2562	2565	2569	rVB2	40601	55952	1.07%	0.166%
23	18.298	2582	2586	2591	rBV3	113420	203219	3.88%	0.603%
24	18.357	2592	2596	2608	rVB3	128463	319917	6.10%	0.950%
25	19.198	2733	2739	2745	rBV	658242	847955	16.17%	2.517%
26	19.339	2757	2763	2773	rBV	537868	849292	16.20%	2.521%
27	19.575	2794	2803	2808	rBV	513433	861516	16.43%	2.557%
28	19.786	2833	2839	2847	rBV	3787522	5242669	100.00%	15.560%
29	20.098	2889	2892	2895	rVB2	61943	69847	1.33%	0.207%
30	20.198	2906	2909	2913	rVB	53305	62490	1.19%	0.185%
31	20.263	2916	2920	2926	rVB4	98857	183811	3.51%	0.546%
32	21.116	3062	3065	3068	rVV2	75825	83234	1.59%	0.247%
33	21.163	3069	3073	3082	rVB4	218033	390402	7.45%	1.159%
34	21.492	3122	3129	3134	rBV2	1275478	2268325	43.27%	6.732%
35	21.539	3135	3137	3152	rVB	290972	484134	9.23%	1.437%
36	23.727	3503	3509	3517	rBV3	288115	876096	16.71%	2.600%

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ClientSampleId :
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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-BP051325.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.457	3628	3633	3642	rVB	159917	352736	6.73%	1.047%
38	24.598	3651	3657	3667	rVB	206151	541755	10.33%	1.608%
39	24.762	3676	3685	3695	rBV2	697123	2071837	39.52%	6.149%

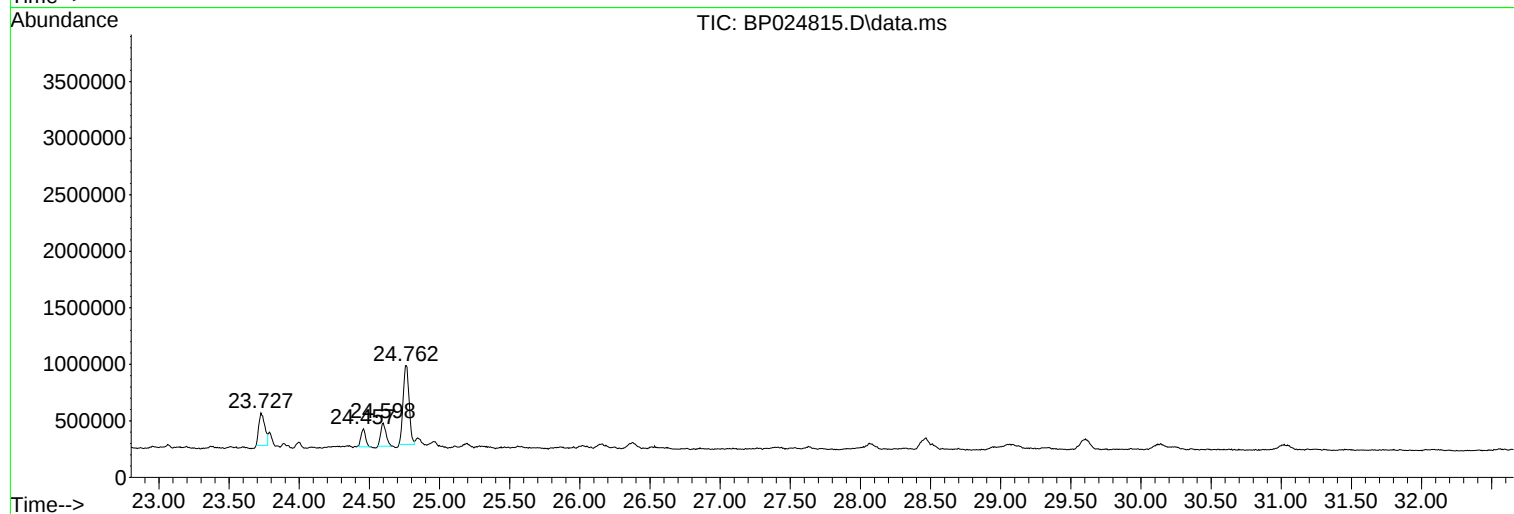
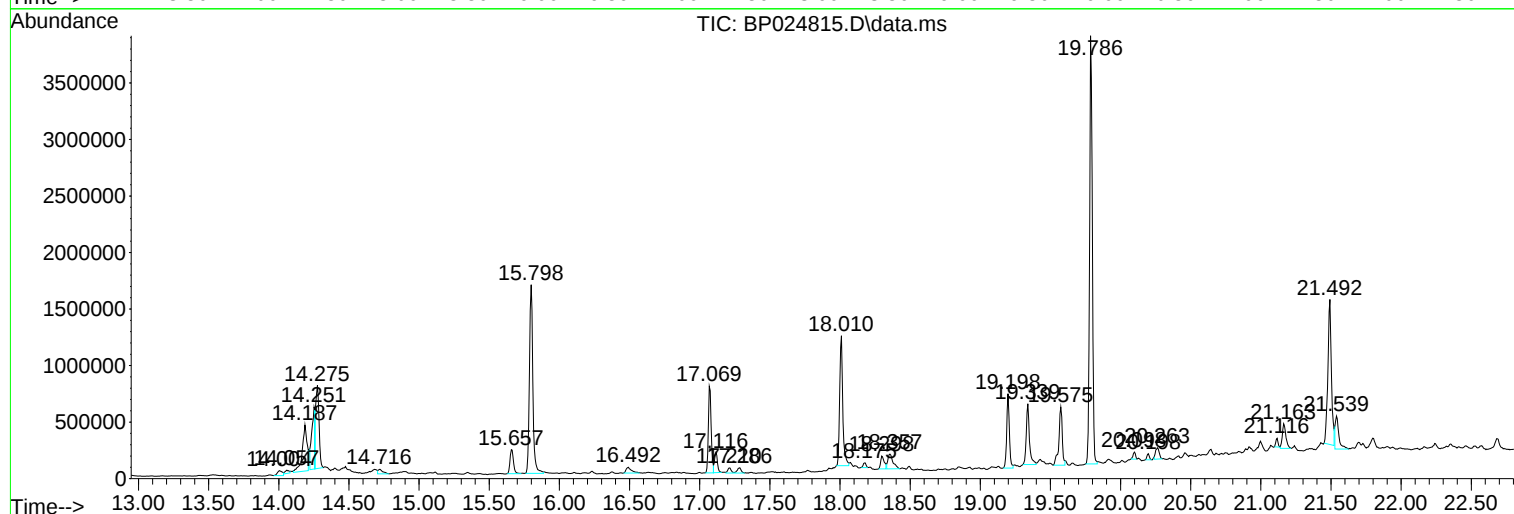
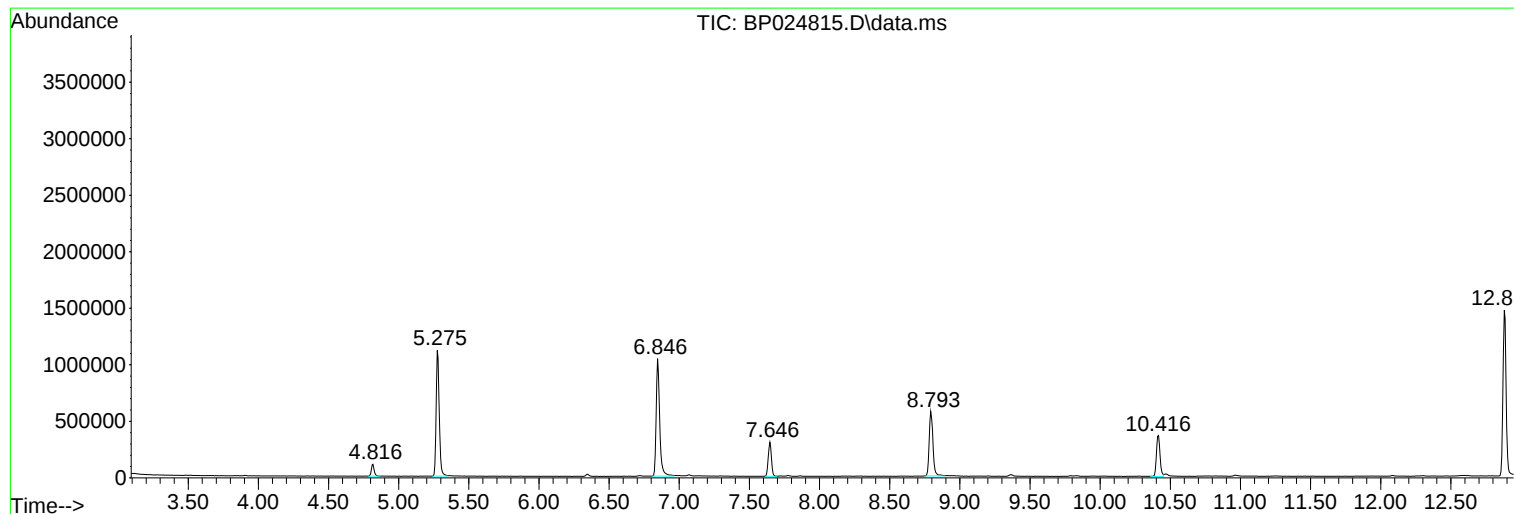
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Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP051325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
Data File : BP024815.D
Acq On : 28 May 2025 14:49
Operator : RC/JU
Sample : Q2128-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

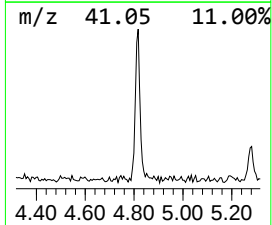
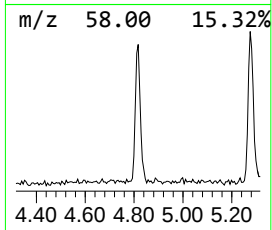
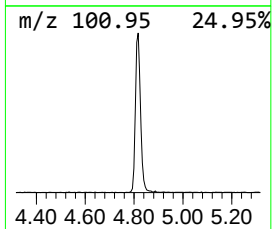
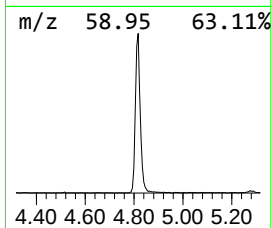
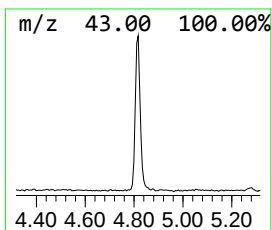
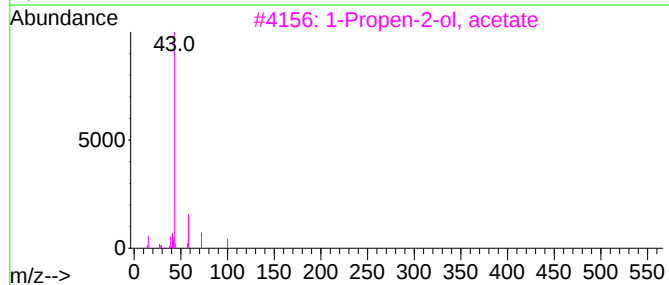
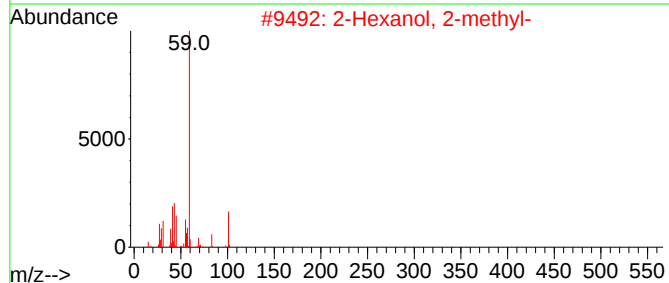
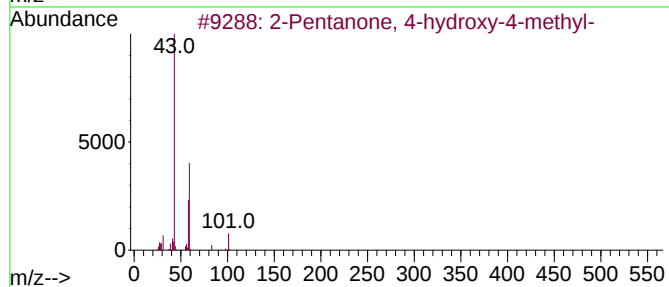
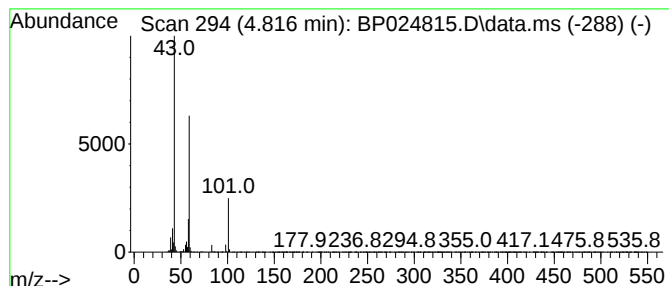
Instrument :
BNA_P
ClientSampleId :
TP03-MHM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP051325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.816	6.50 ng	151761	1,4-Dichlorobenzene-d4	7.646	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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Misc :
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Instrument :
BNA_P
ClientSampleId :
TP03-MHM

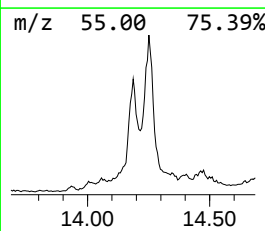
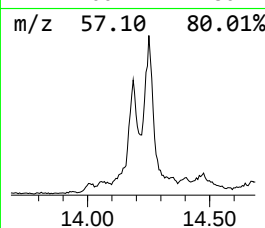
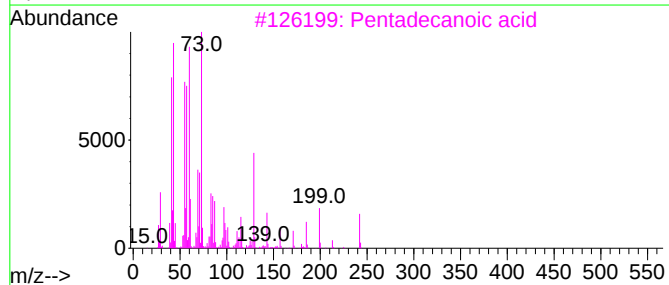
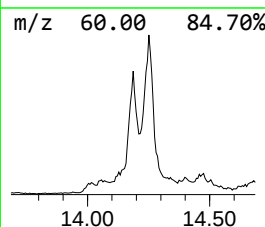
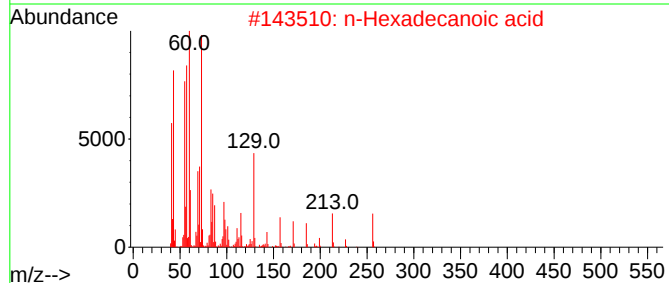
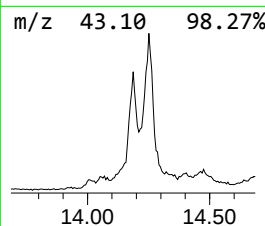
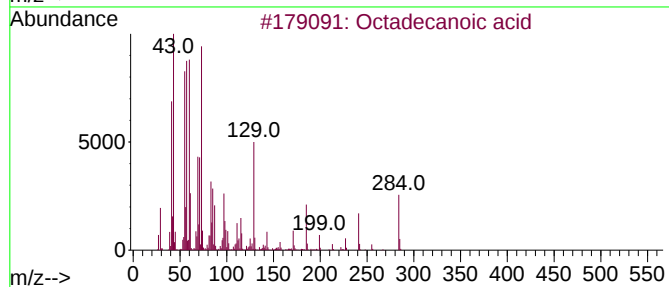
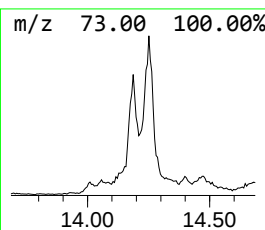
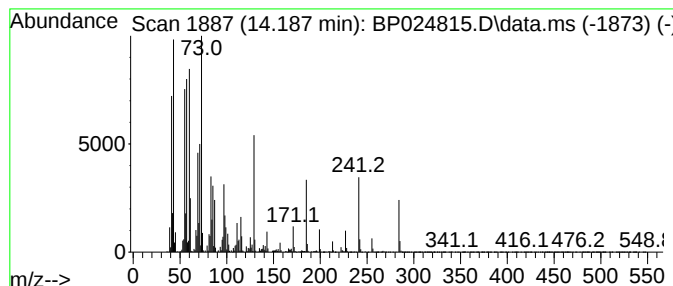
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.187	16.65 ng	979635	Acenaphthene-d10	14.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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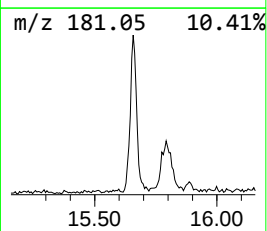
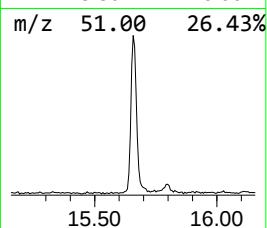
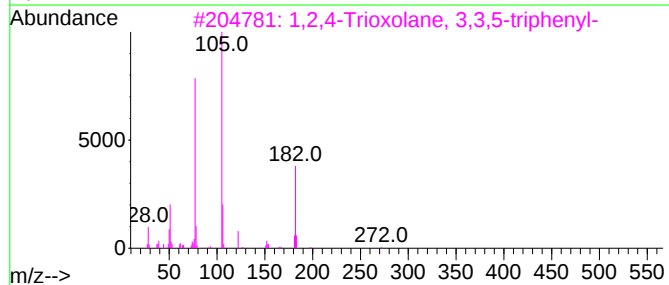
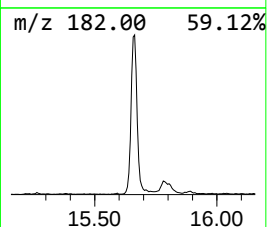
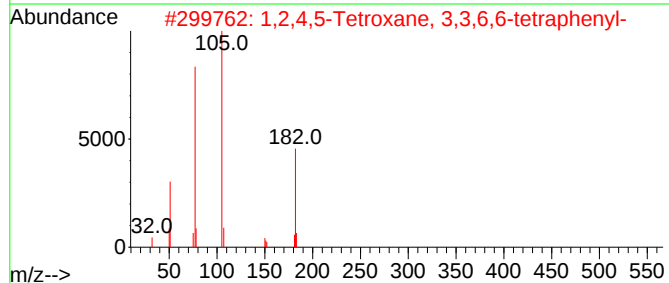
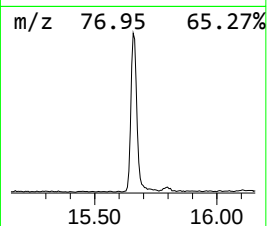
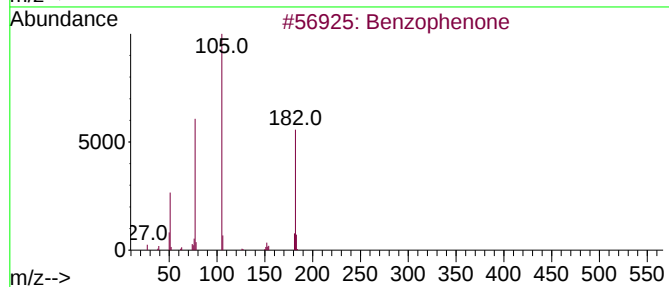
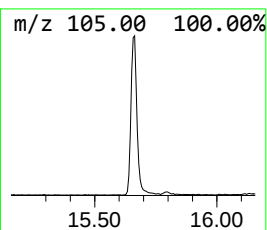
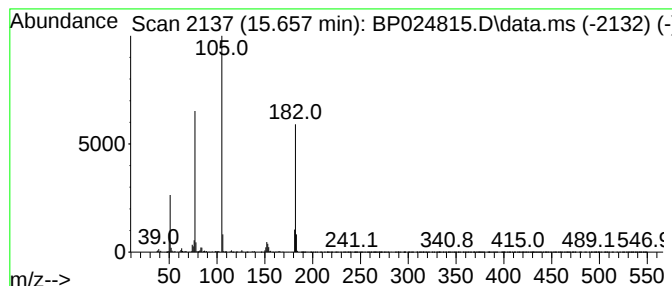
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.657	6.23 ng	366766	Acenaphthene-d10	14.275

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			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
5			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	53



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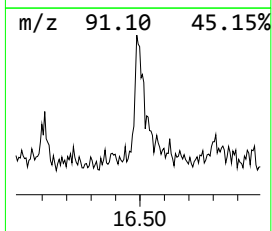
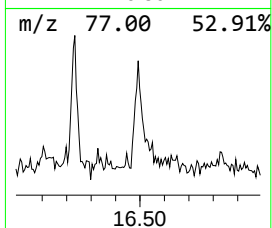
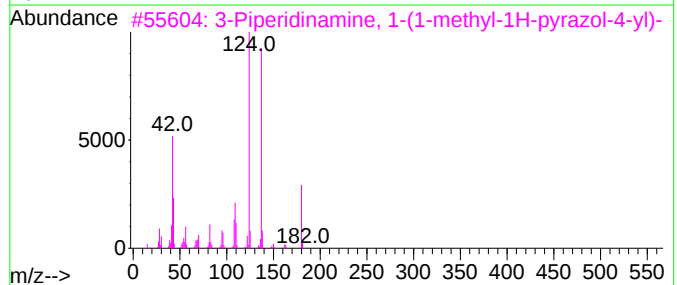
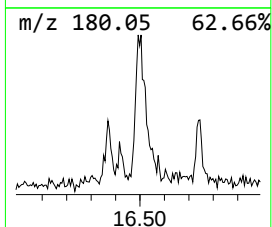
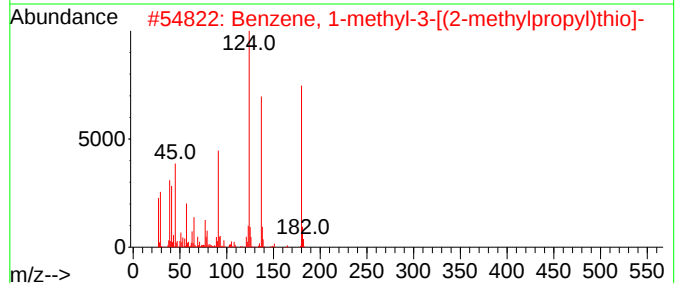
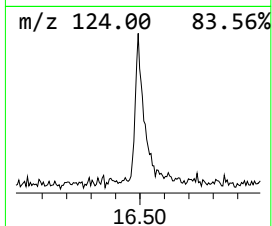
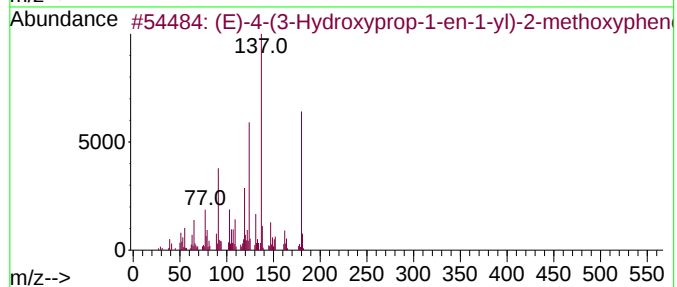
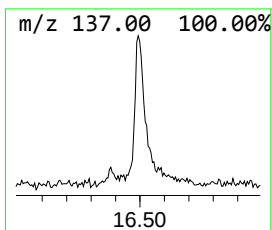
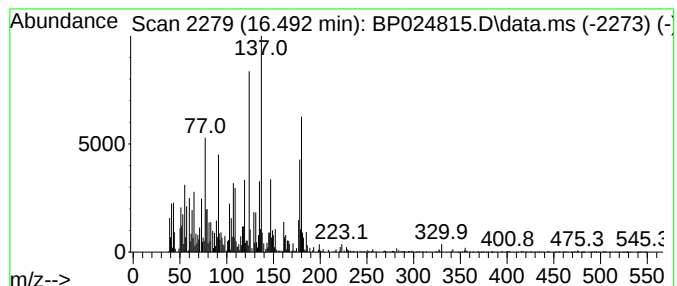
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (E)-4-(3-Hydroxyprop-1-en-1-yl) Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.492	2.58 ng	136867	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	68		
2	Benzene, 1-methyl-3-[(2-methylpr...	180	C11H16S	054576-36-2	46		
3	3-Piperidinamine, 1-(1-methyl-1H...	180	C9H16N4	1251330-45-6	46		
4	Benzene, 1-methyl-4-[(2-methylpr...	180	C11H16S	054576-37-3	41		
5	3-Piperidinamine, 1-(1-methyl-1H...	252	C12H24N4Si	1000470-29-5	38		



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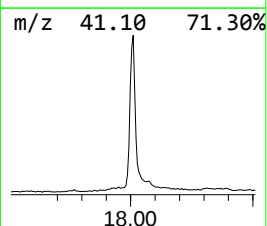
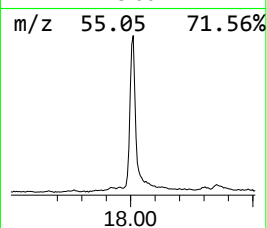
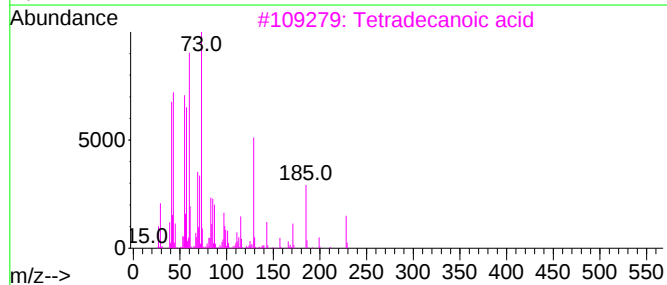
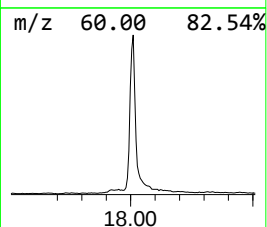
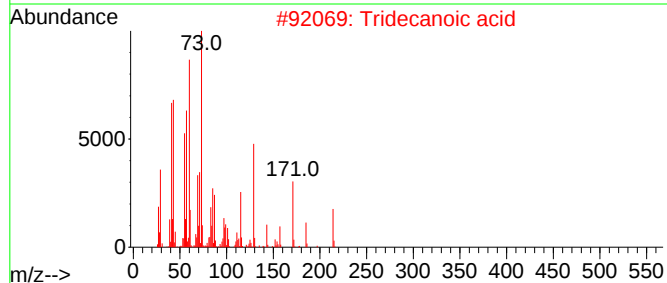
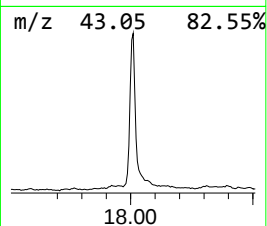
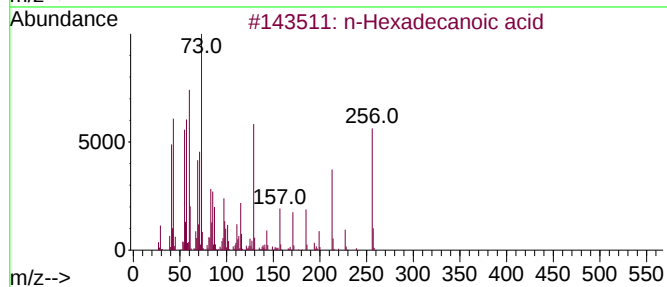
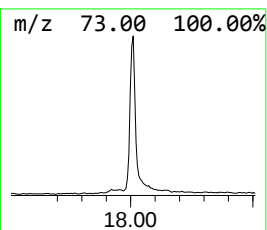
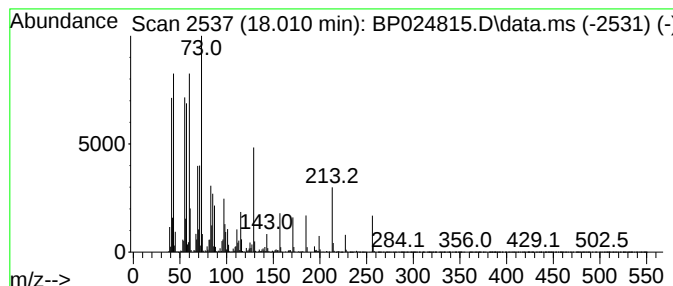
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.010	33.29 ng	1763330	Phenanthrene-d10		17.069	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
5	Undecanoic acid		186	C11H22O2	000112-37-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
Data File : BP024815.D
Acq On : 28 May 2025 14:49
Operator : RC/JU
Sample : Q2128-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

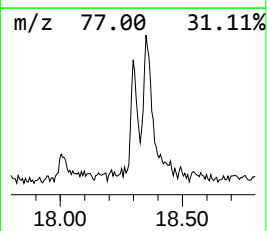
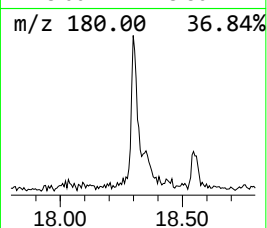
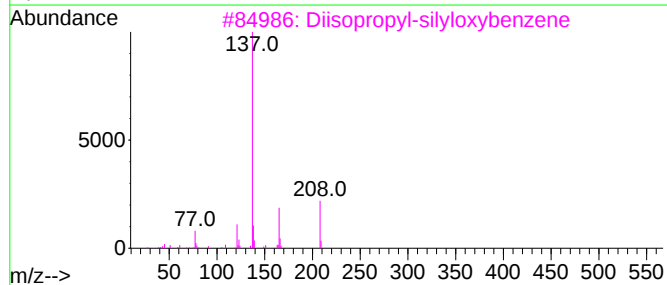
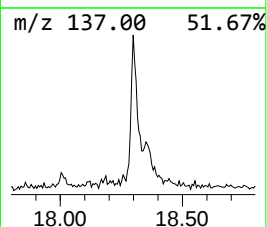
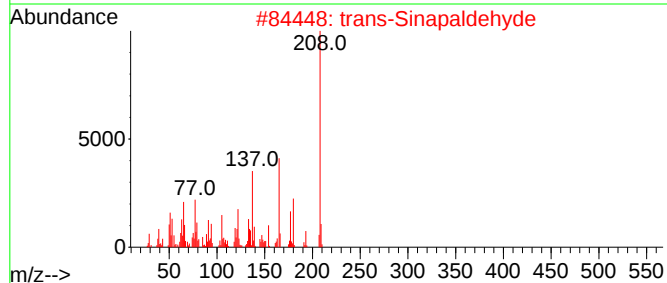
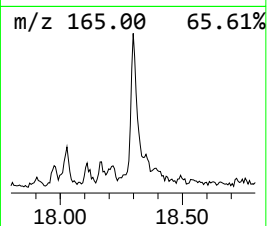
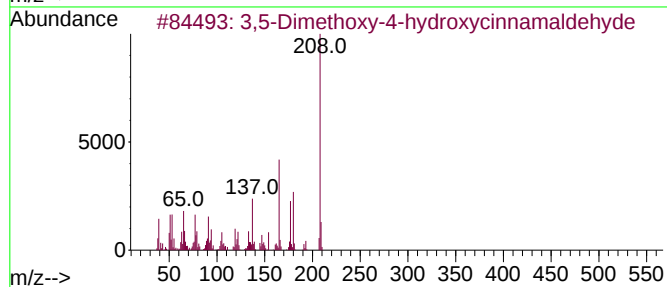
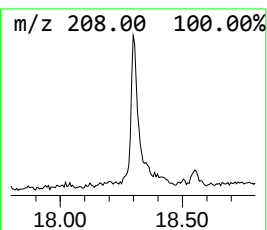
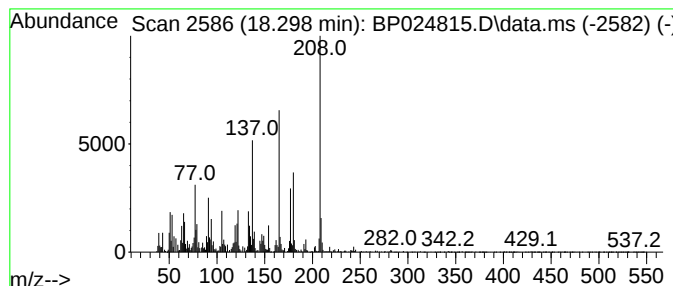
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ClientSampleId :
TP03-MHM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP051325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.298	3.84 ng	203219	Phenanthrene-d10		17.069	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...		208	C11H12O4	087345-53-7	96
2	trans-Sinapaldehyde		208	C11H12O4	004206-58-0	93
3	Diisopropyl-silyloxybenzene		208	C12H20OSi	1000292-68-7	49
4	Imidazo[5,4-e][1,4]diazepine-4,7...		208	C9H12N4O2	144105-22-6	49
5	3-tert-Butyl-4-hydroxyanisole		180	C11H16O2	000121-00-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
Data File : BP024815.D
Acq On : 28 May 2025 14:49
Operator : RC/JU
Sample : Q2128-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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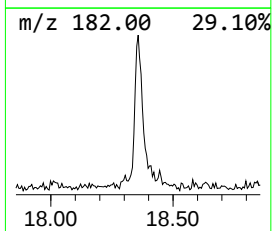
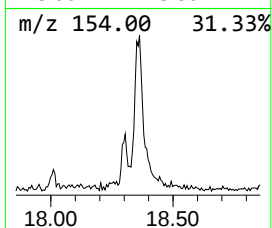
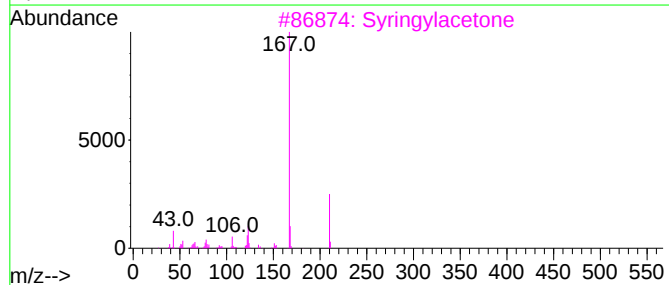
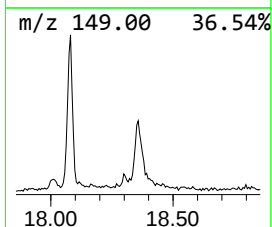
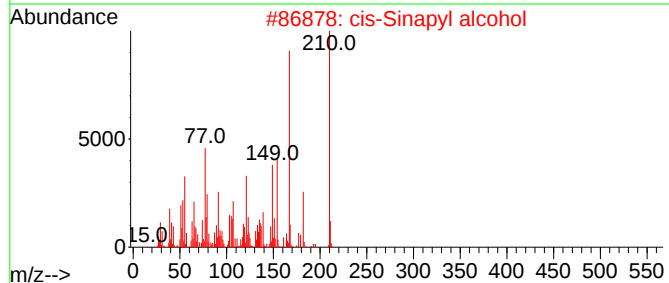
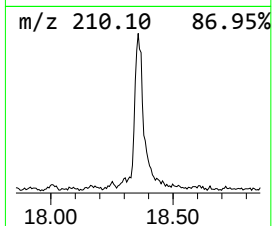
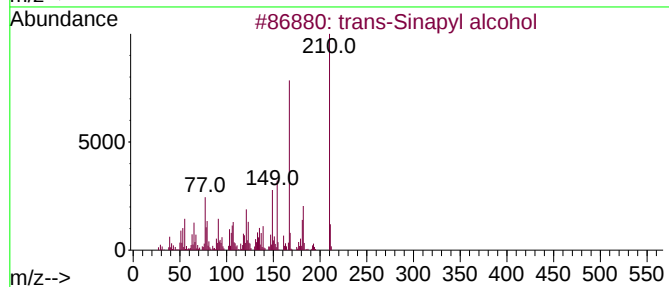
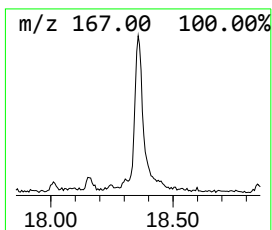
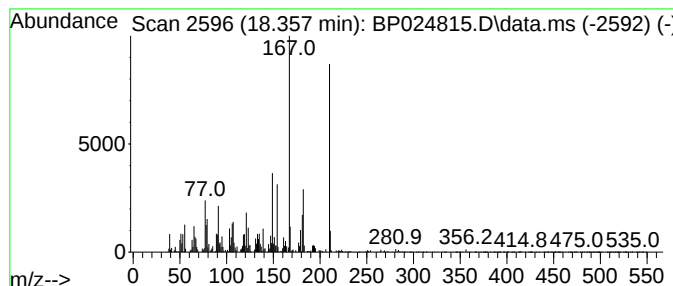
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 trans-Sinapyl alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.357	6.04 ng	319917	Phenanthrene-d10	17.069

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	74
3		Syringylacetone	210	C11H14O4	019037-58-2	58
4		Altretamine	210	C9H18N6	000645-05-6	38
5		9-Methyl-1-phenazinol	210	C13H10N2O	013860-43-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
Data File : BP024815.D
Acq On : 28 May 2025 14:49
Operator : RC/JU
Sample : Q2128-01
Misc :
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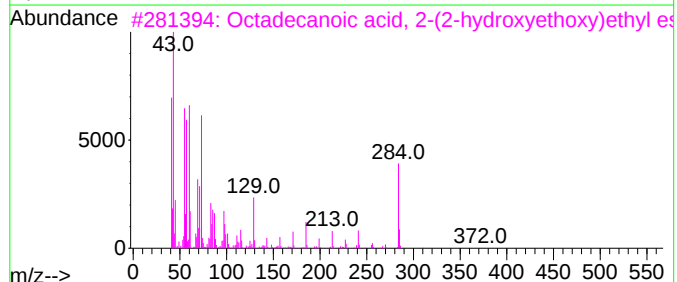
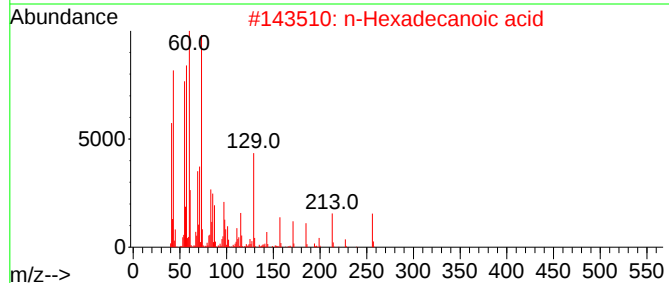
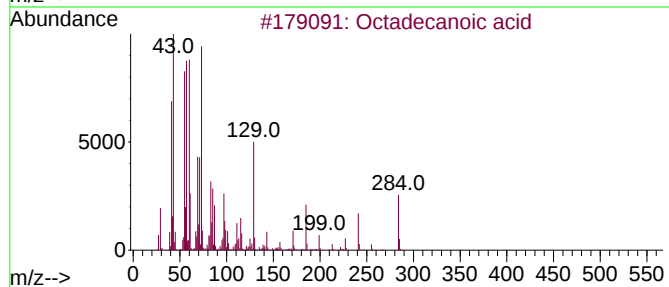
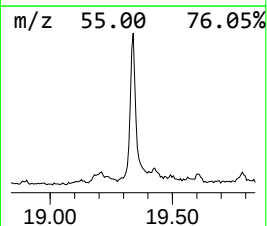
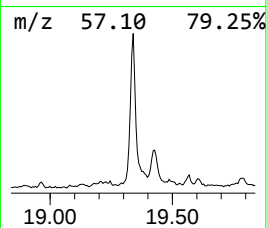
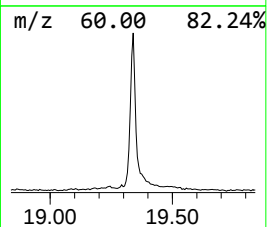
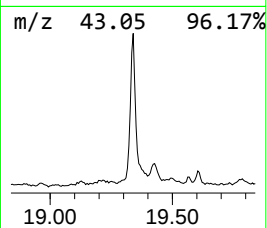
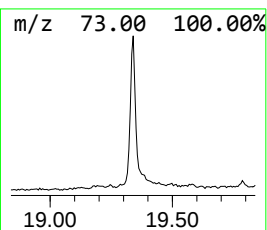
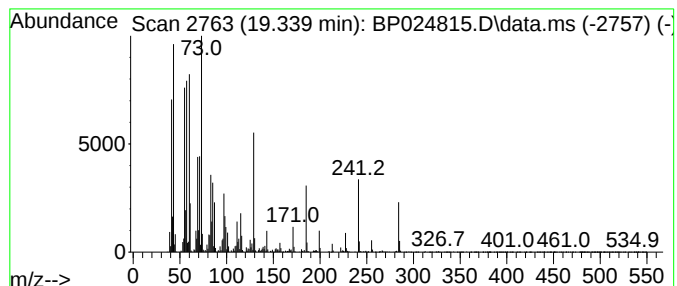
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP051325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, 2-(2-hyd... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.339	7.49 ng	849292	Chrysene-d12	21.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
Data File : BP024815.D
Acq On : 28 May 2025 14:49
Operator : RC/JU
Sample : Q2128-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP03-MHM

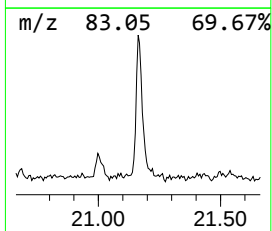
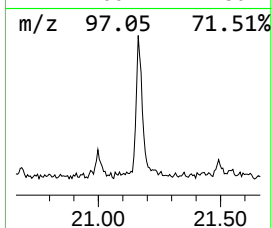
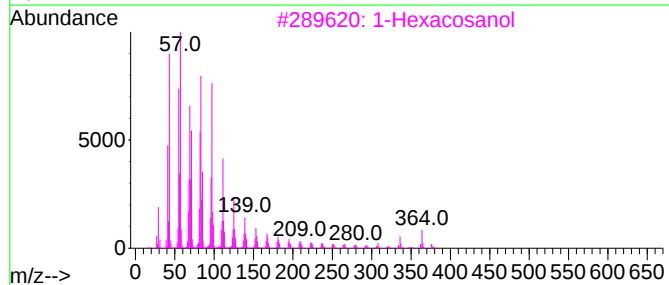
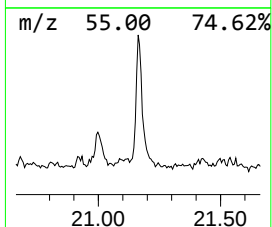
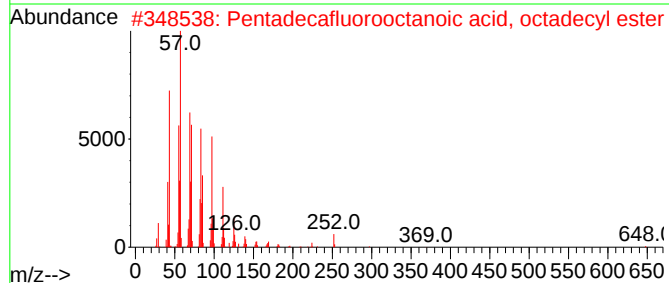
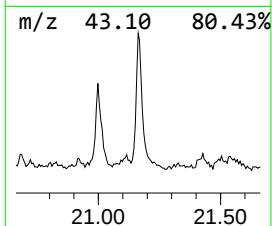
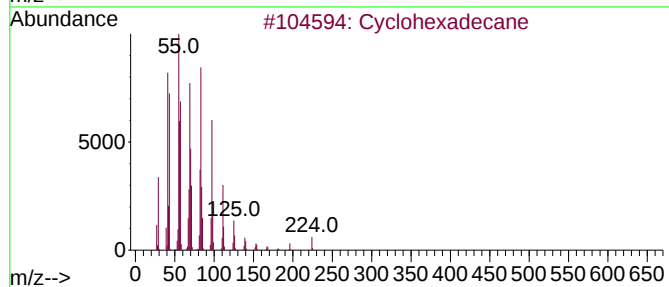
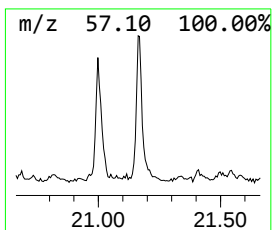
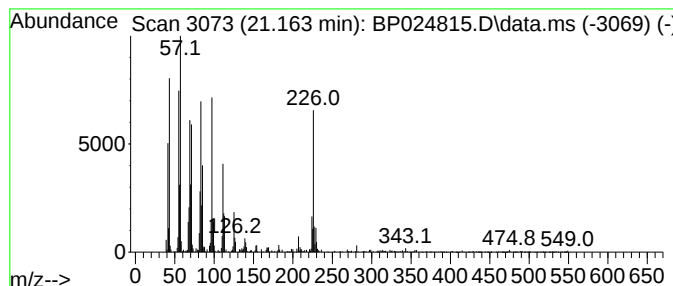
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.163	3.44 ng	390402	Chrysene-d12	21.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	96
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			1-Hexacosanol	382	C26H54O	000506-52-5	90
4			17-Pentatriacontene	491	C35H70	006971-40-0	90
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
Data File : BP024815.D
Acq On : 28 May 2025 14:49
Operator : RC/JU
Sample : Q2128-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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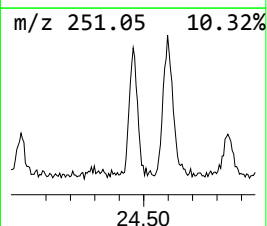
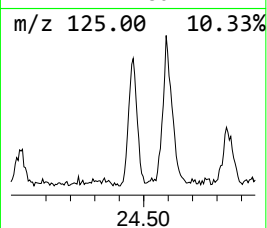
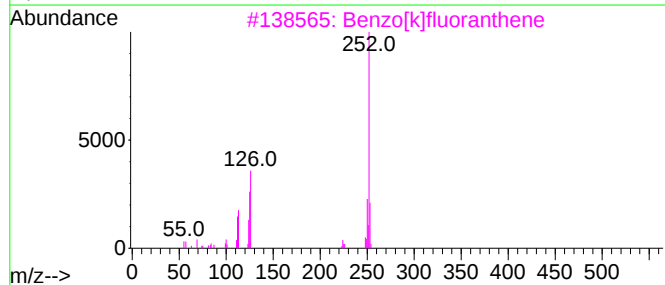
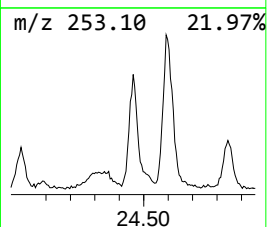
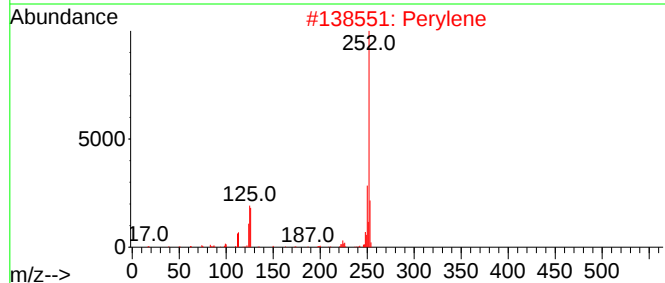
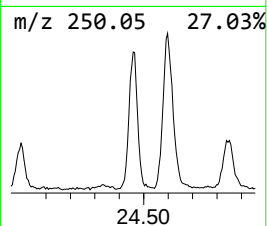
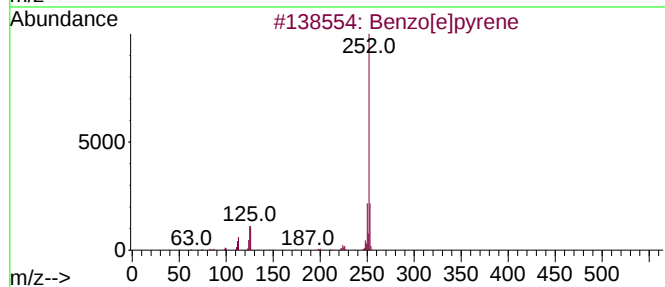
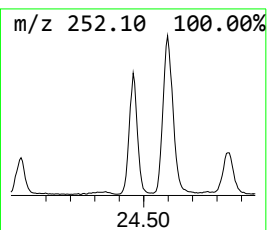
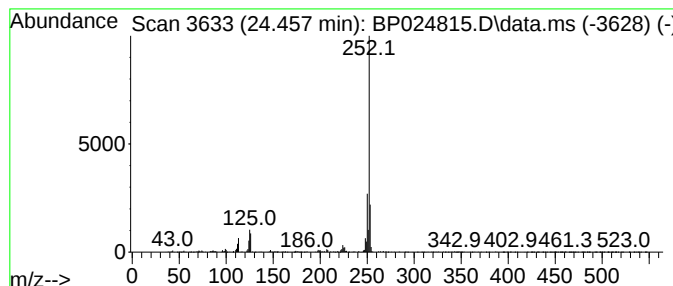
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.457	3.41 ng	352736	Perylene-d12	24.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Perylene	252	C20H12	000198-55-0	94
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP052825\
Data File : BP024815.D
Acq On : 28 May 2025 14:49
Operator : RC/JU
Sample : Q2128-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP03-MHM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP051325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.816	6.5	ng	151761	1	7.646	466782	20.0
Octadecanoic acid	14.187	16.6	ng	979635	3	14.275	1176730	20.0
Benzophenone	15.657	6.2	ng	366766	3	14.275	1176730	20.0
(E)-4-(3-Hydrox...	16.492	2.6	ng	136867	4	17.069	1059270	20.0
n-Hexadecanoic ...	18.010	33.3	ng	1763330	4	17.069	1059270	20.0
3,5-Dimethoxy-4...	18.298	3.8	ng	203219	4	17.069	1059270	20.0
trans-Sinapyl a...	18.357	6.0	ng	319917	4	17.069	1059270	20.0
Octadecanoic ac...	19.339	7.5	ng	849292	5	21.492	2268330	20.0
Cyclohexadecane	21.163	3.4	ng	390402	5	21.492	2268330	20.0
Benzo[e]pyrene	24.457	3.4	ng	352736	6	24.762	2071840	20.0