

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
 Data File : BP025387.D
 Acq On : 13 Aug 2025 16:50
 Operator : CG/JU
 Sample : Q2820-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 82H-N

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: BP025387.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.967	3	5	13	rVB2	167776	222164	3.27%	0.573%
2	3.043	13	18	31	rVB	1085809	1294033	19.05%	3.337%
3	4.949	336	342	350	rBV	183730	249888	3.68%	0.644%
4	5.408	413	420	431	rBV	1886325	2731582	40.22%	7.045%
5	6.966	677	685	695	rBV	1687169	2666716	39.27%	6.878%
6	7.796	818	826	833	rVB	598275	1015496	14.95%	2.619%
7	8.931	1012	1019	1028	rBV	1136494	1867484	27.50%	4.816%
8	10.566	1289	1297	1307	rBV	793999	1367039	20.13%	3.526%
9	13.025	1707	1715	1728	rBV	2888975	4322261	63.64%	11.147%
10	14.413	1941	1951	1959	rBV	1107973	1747225	25.73%	4.506%
11	15.789	2178	2185	2194	rBV	233933	343374	5.06%	0.886%
12	15.925	2201	2208	2226	rBV	2048481	3297544	48.55%	8.505%
13	16.366	2278	2283	2287	rVB	56824	78884	1.16%	0.203%
14	17.207	2419	2426	2432	rBV2	1264738	2102008	30.95%	5.421%
15	18.154	2582	2587	2595	rBV	642572	968366	14.26%	2.497%
16	19.330	2782	2787	2796	rBV	227131	377443	5.56%	0.973%
17	19.478	2808	2812	2819	rBV2	201171	300145	4.42%	0.774%
18	19.707	2844	2851	2856	rBV	210637	351992	5.18%	0.908%
19	19.930	2882	2889	2897	rBV	4669019	6791392	100.00%	17.515%
20	21.336	3123	3128	3137	rVB	522711	767081	11.29%	1.978%
21	21.666	3176	3184	3189	rBV	1617723	2969322	43.72%	7.658%
22	25.065	3753	3762	3774	rVB	1102303	2942188	43.32%	7.588%

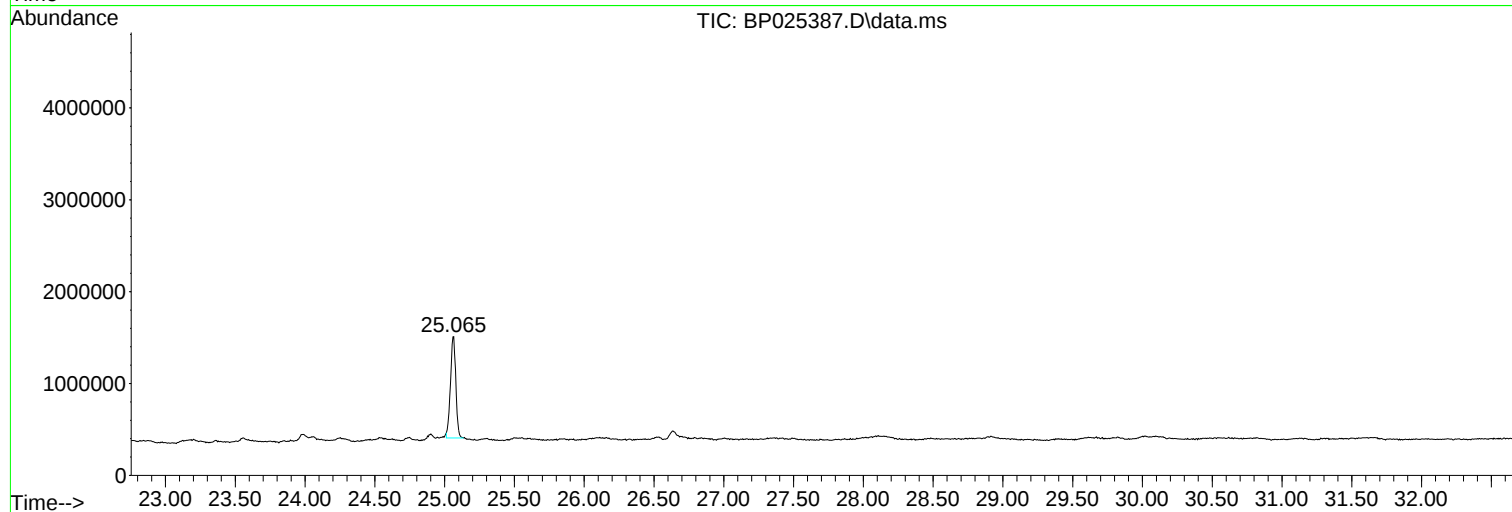
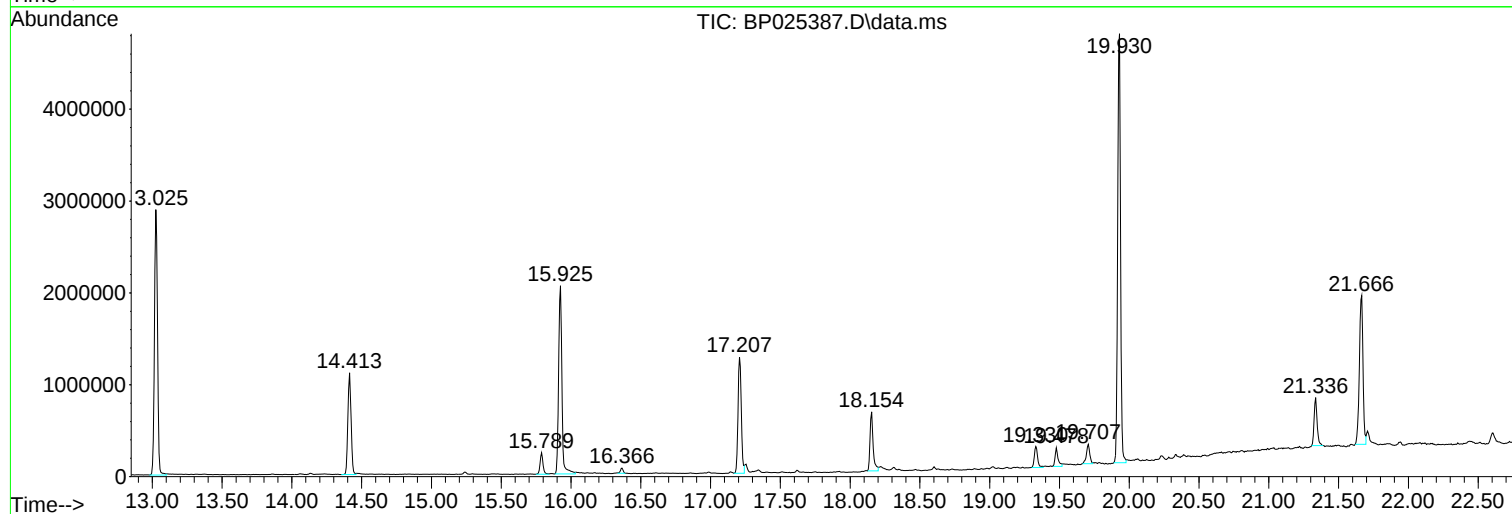
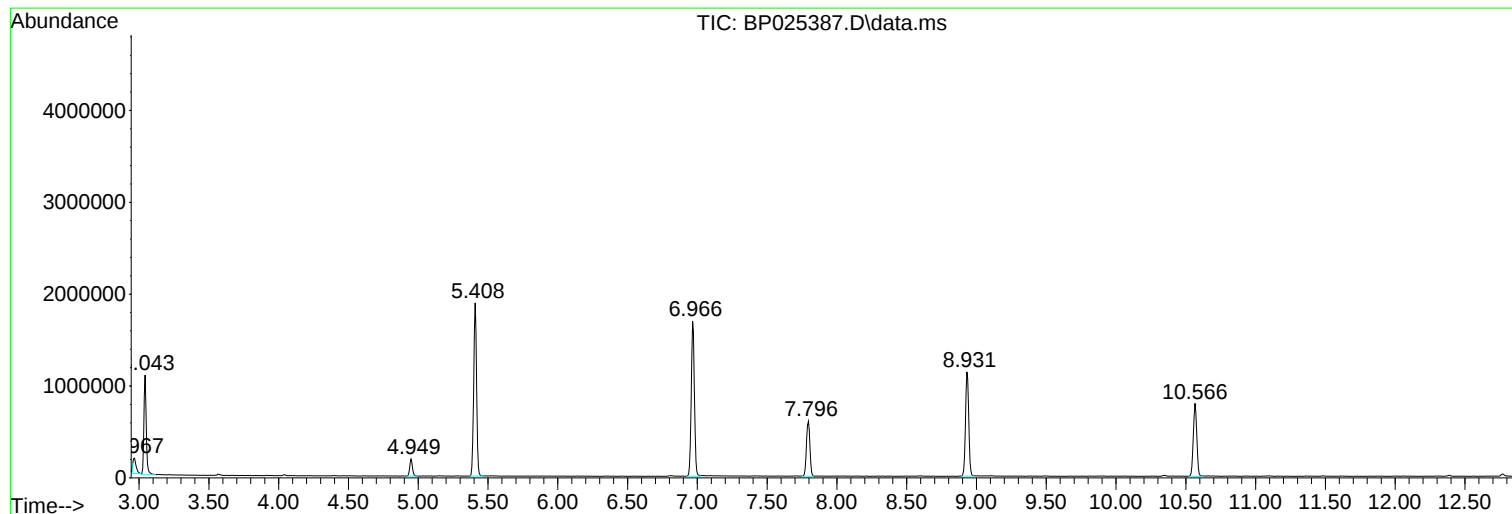
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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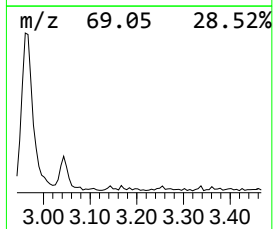
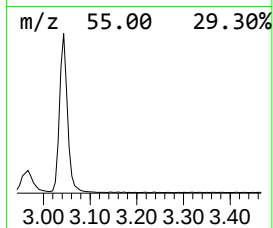
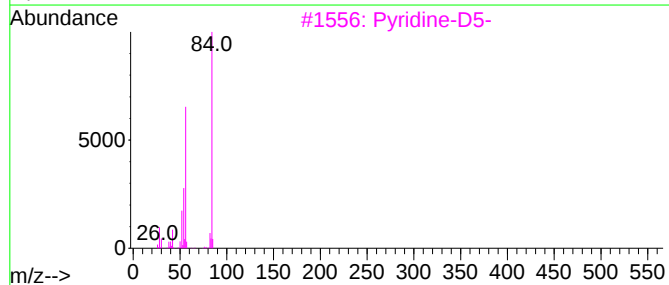
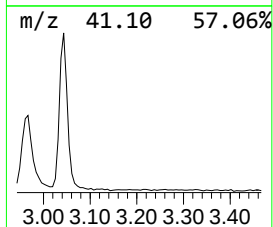
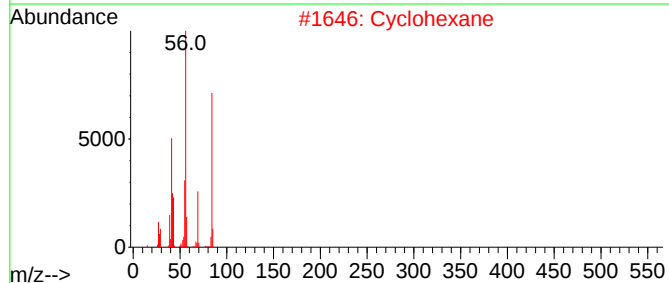
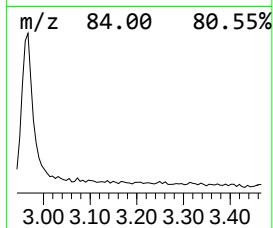
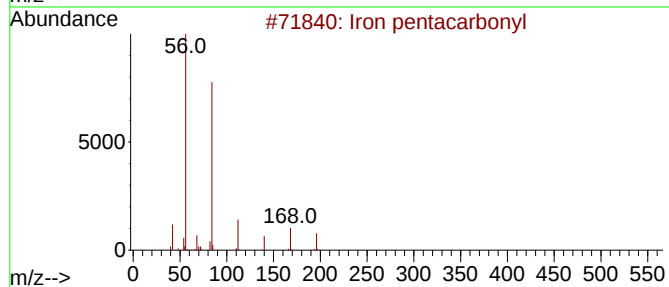
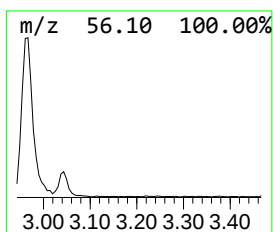
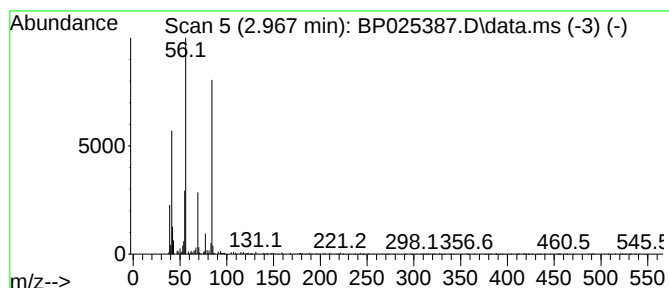
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Iron pentacarbonyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.967	4.38 ng	222164	1,4-Dichlorobenzene-d4	7.796

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Iron pentacarbonyl	196	C5FeO5	013463-40-6	78
2		Cyclohexane	84	C6H12	000110-82-7	72
3		Pyridine-D5-	84	C5D5N	007291-22-7	56
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	50
5		2-Piperidinemethanol	115	C6H13NO	003433-37-2	43



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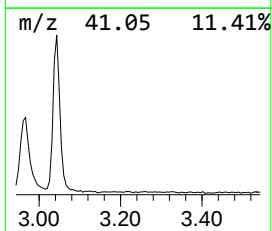
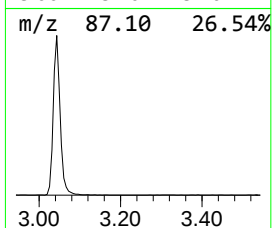
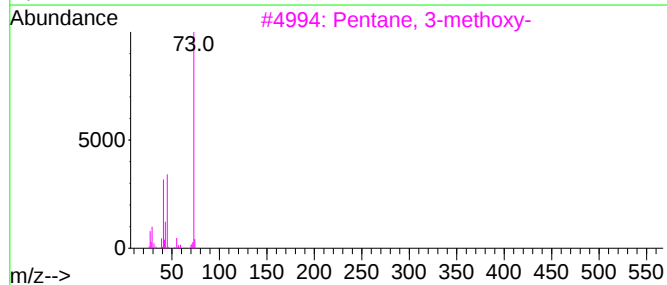
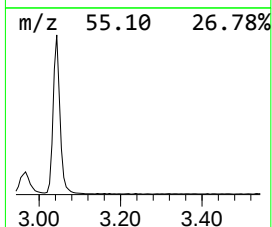
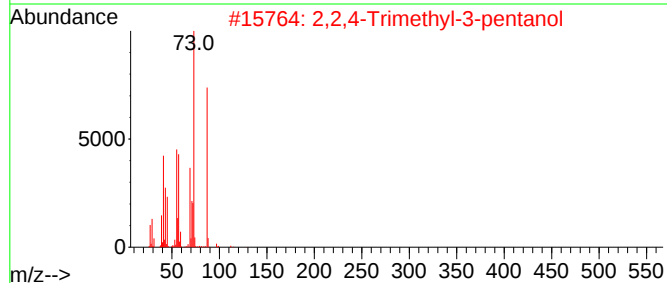
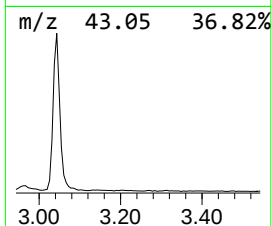
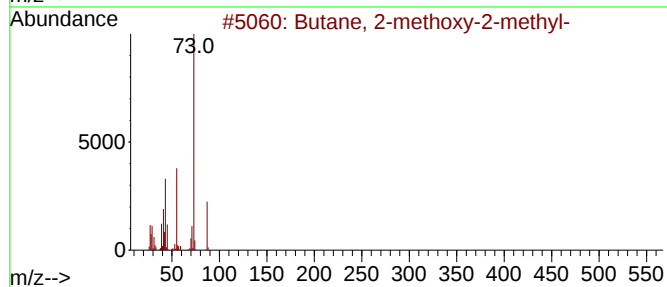
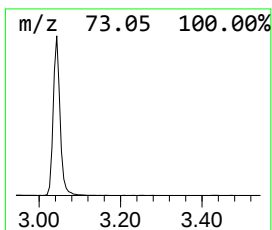
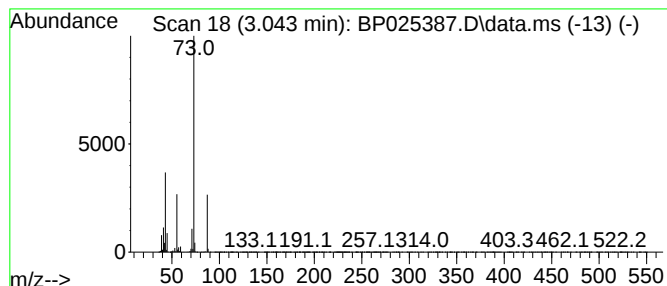
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.043	25.49 ng	1294030	1,4-Dichlorobenzene-d4	7.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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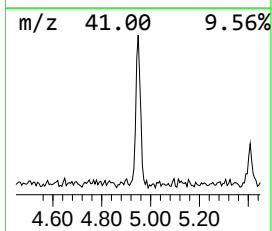
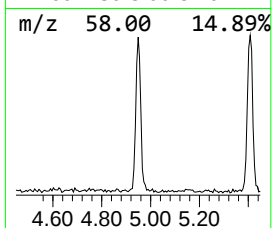
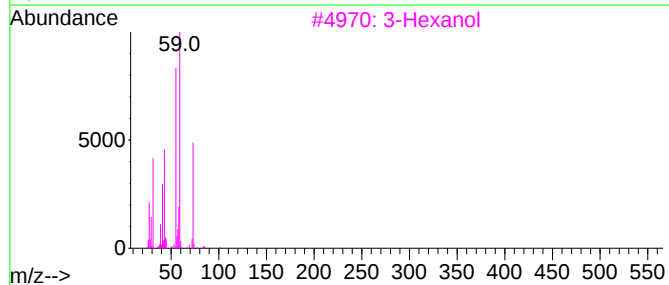
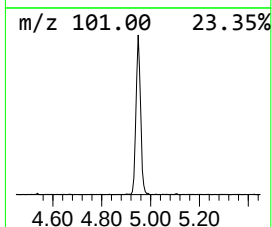
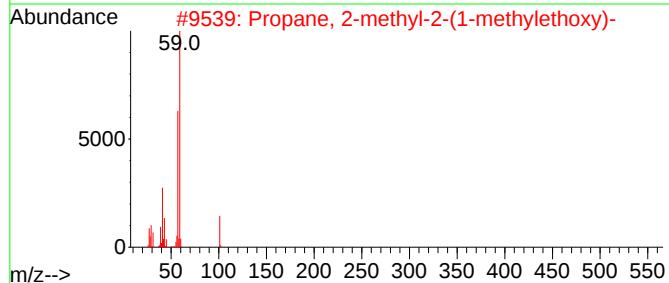
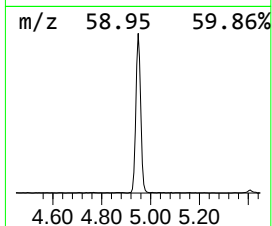
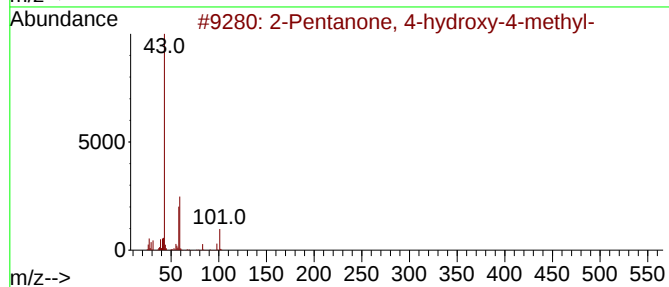
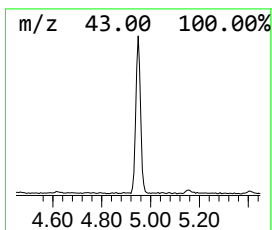
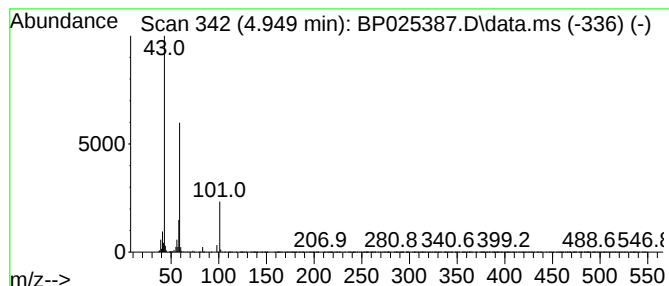
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.949	4.92 ng	249888	1,4-Dichlorobenzene-d4	7.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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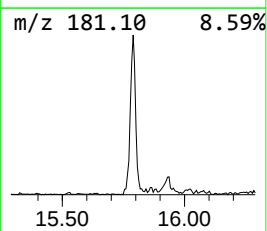
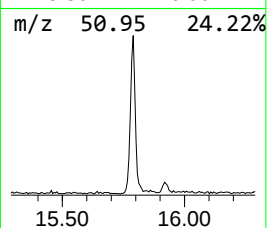
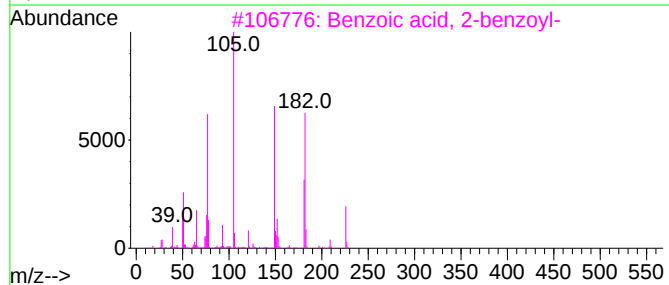
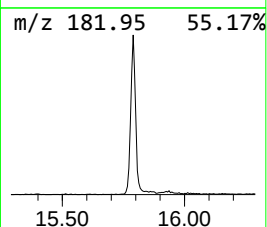
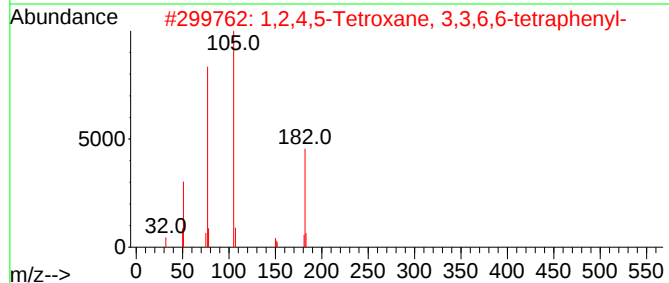
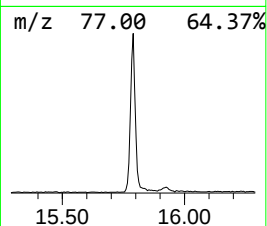
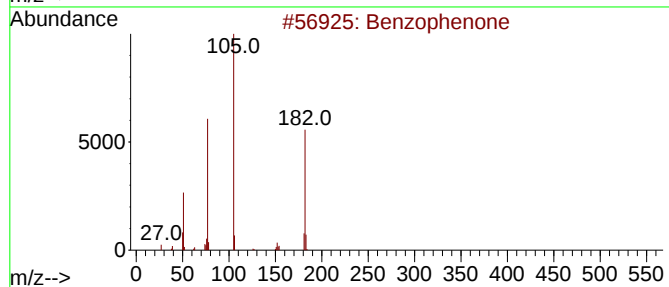
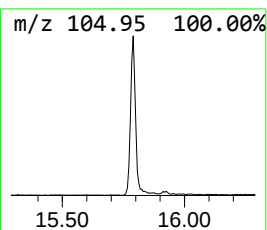
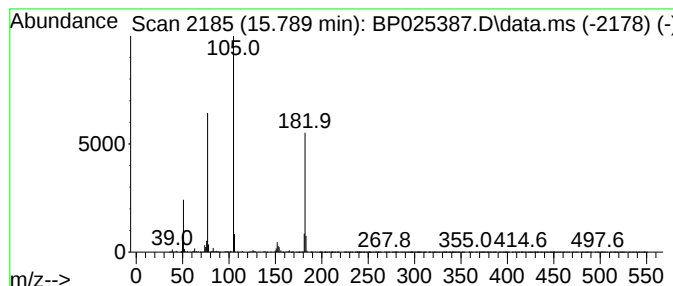
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Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.790	3.93 ng	343374	Acenaphthene-d10	14.413

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			Benzoic acid, 2-benzoyl-	226	C14H10O3	000085-52-9	56
4			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
5			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50



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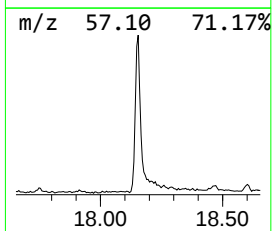
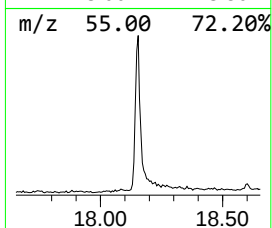
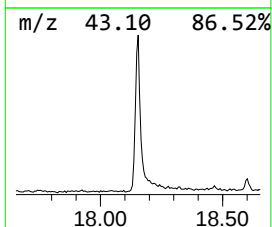
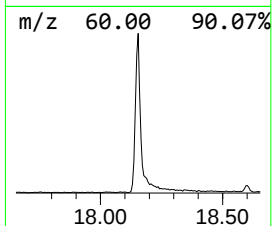
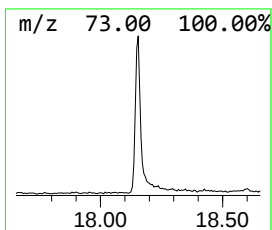
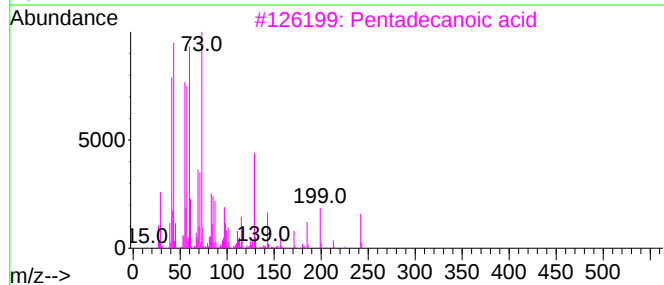
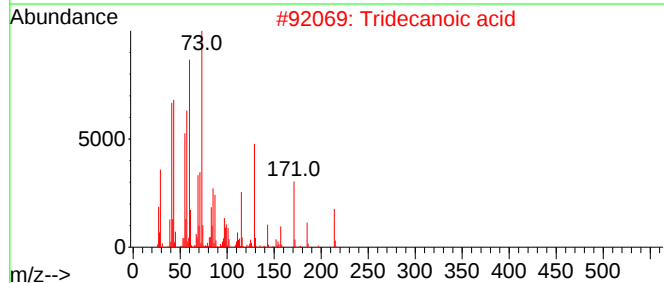
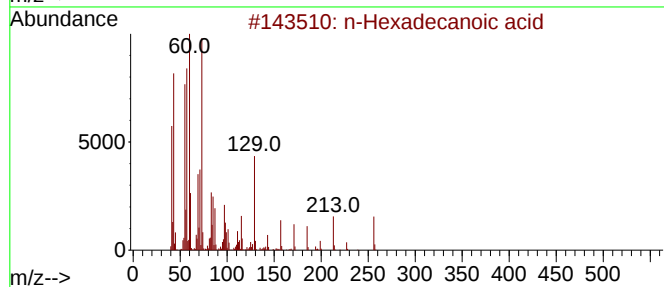
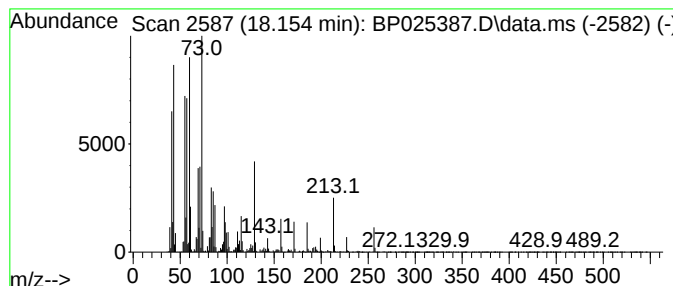
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.154	9.21 ng	968366	Phenanthrene-d10	17.207

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	80



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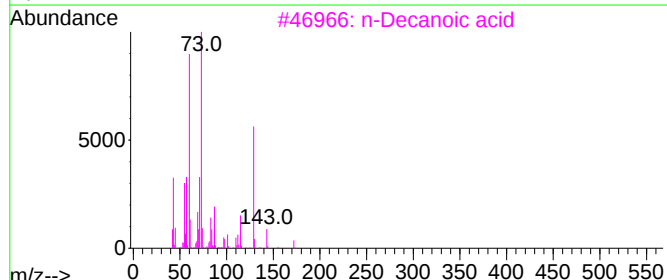
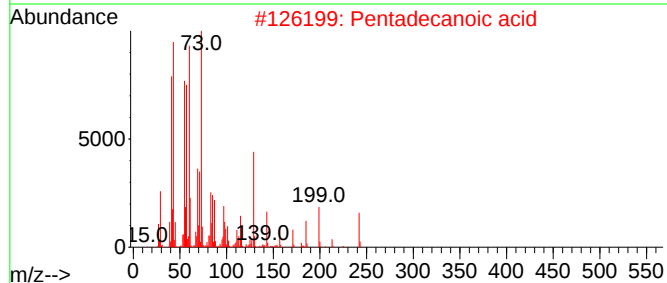
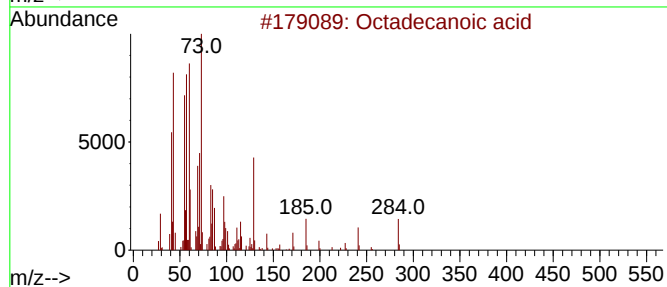
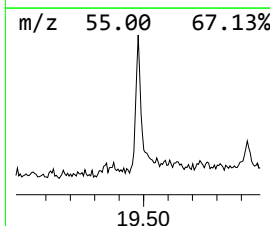
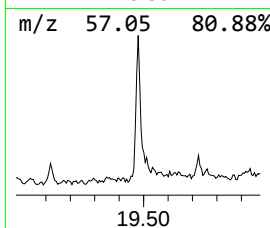
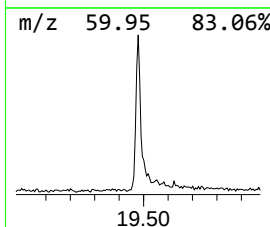
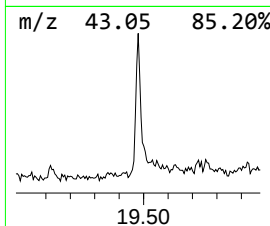
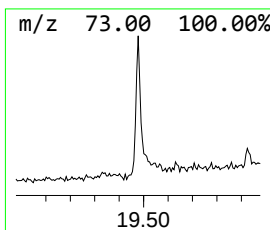
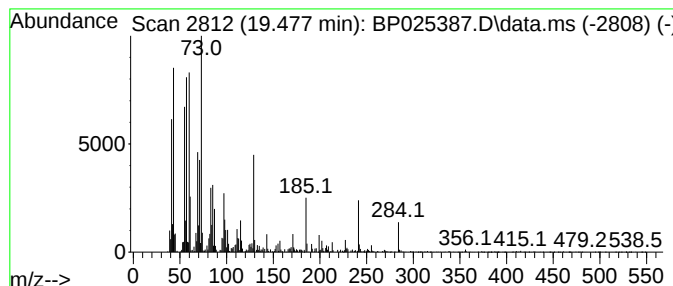
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.477	2.02 ng	300145	Chrysene-d12	21.666

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Decanoic acid	172	C10H20O2	000334-48-5	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025387.D
Acq On : 13 Aug 2025 16:50
Operator : CG/JU
Sample : Q2820-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
82H-N

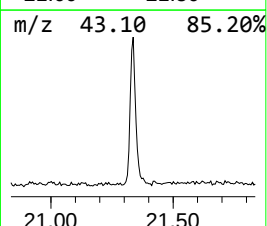
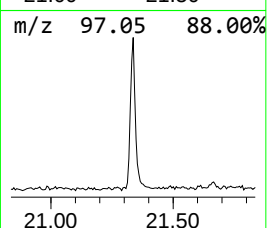
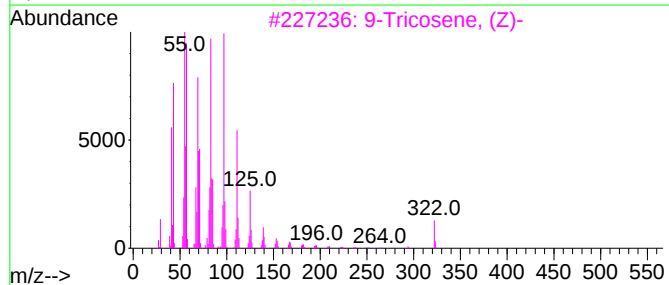
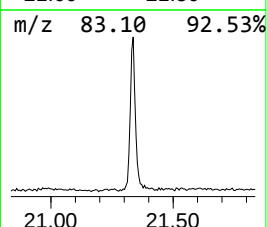
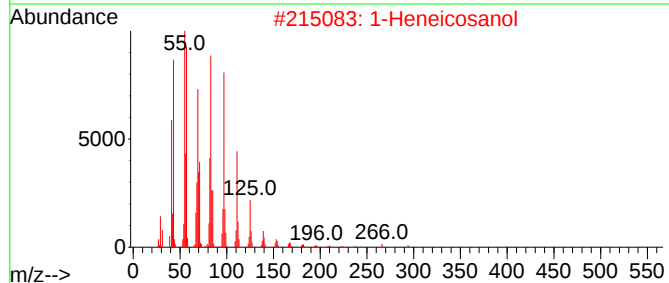
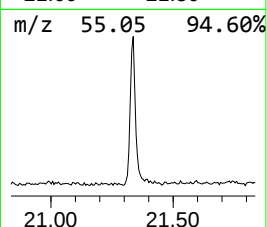
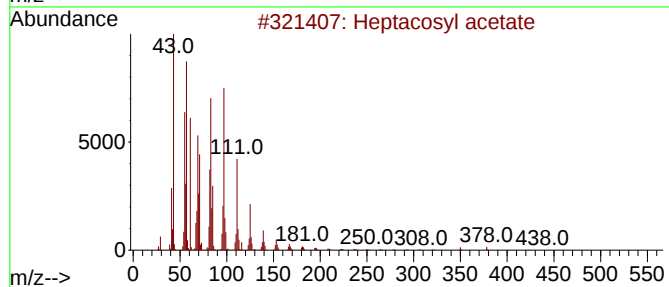
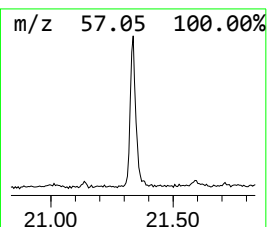
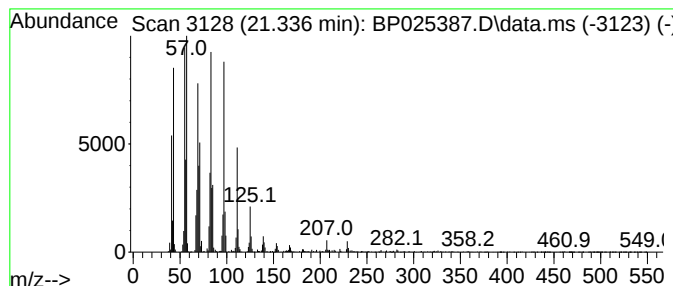
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.336	5.17 ng	767081	Chrysene-d12	21.666

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	96
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081325\
Data File : BP025387.D
Acq On : 13 Aug 2025 16:50
Operator : CG/JU
Sample : Q2820-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
82H-N

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
Iron pentacarbonyl	2.967	4.4	ng	222164	1	7.796	1015500	20.0
Butane, 2-metho...	3.043	25.5	ng	1294030	1	7.796	1015500	20.0
2-Pentanone, 4-...	4.949	4.9	ng	249888	1	7.796	1015500	20.0
Benzophenone	15.790	3.9	ng	343374	3	14.413	1747230	20.0
n-Hexadecanoic ...	18.154	9.2	ng	968366	4	17.207	2102010	20.0
Octadecanoic acid	19.477	2.0	ng	300145	5	21.666	2969320	20.0
Heptacosyl acetate	21.336	5.2	ng	767081	5	21.666	2969320	20.0