

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP050625\
 Data File : BP024550.D
 Acq On : 06 May 2025 17:08
 Operator : RC/JU
 Sample : Q1956-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB2-4-5

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	298	304	314	rBV	205233	292378	3.70%	0.694%
2	5.328	375	381	397	rBV	2297393	3427916	43.32%	8.136%
3	6.893	640	647	669	rBV	2238787	3544190	44.79%	8.412%
4	7.704	777	785	792	rBV	518080	842897	10.65%	2.000%
5	8.851	972	980	998	rBV	1378223	2293143	28.98%	5.442%
6	10.475	1249	1256	1270	rBV	662078	1179116	14.90%	2.798%
7	12.945	1668	1676	1696	rBV	3407716	5208455	65.82%	12.361%
8	14.333	1905	1912	1927	rBV	1103294	1578282	19.95%	3.746%
9	14.563	1942	1951	1969	rBV	1153667	2513156	31.76%	5.965%
10	14.945	2004	2016	2017	rBV	69536	179533	2.27%	0.426%
11	15.716	2141	2147	2154	rBV	226517	336354	4.25%	0.798%
12	15.851	2162	2170	2186	rBV	3091393	4919744	62.17%	11.676%
13	17.139	2382	2389	2395	rBV	1277524	1859389	23.50%	4.413%
14	18.074	2543	2548	2565	rBV	425533	755934	9.55%	1.794%
15	19.404	2770	2774	2785	rBV	90664	175864	2.22%	0.417%
16	19.862	2846	2852	2861	rBV	6713921	7912788	100.00%	18.780%
17	21.256	3084	3089	3101	rBV3	109238	304021	3.84%	0.722%
18	21.580	3138	3144	3162	rVB	1434959	2306734	29.15%	5.475%
19	24.927	3704	3713	3727	rVB	875912	2505030	31.66%	5.945%

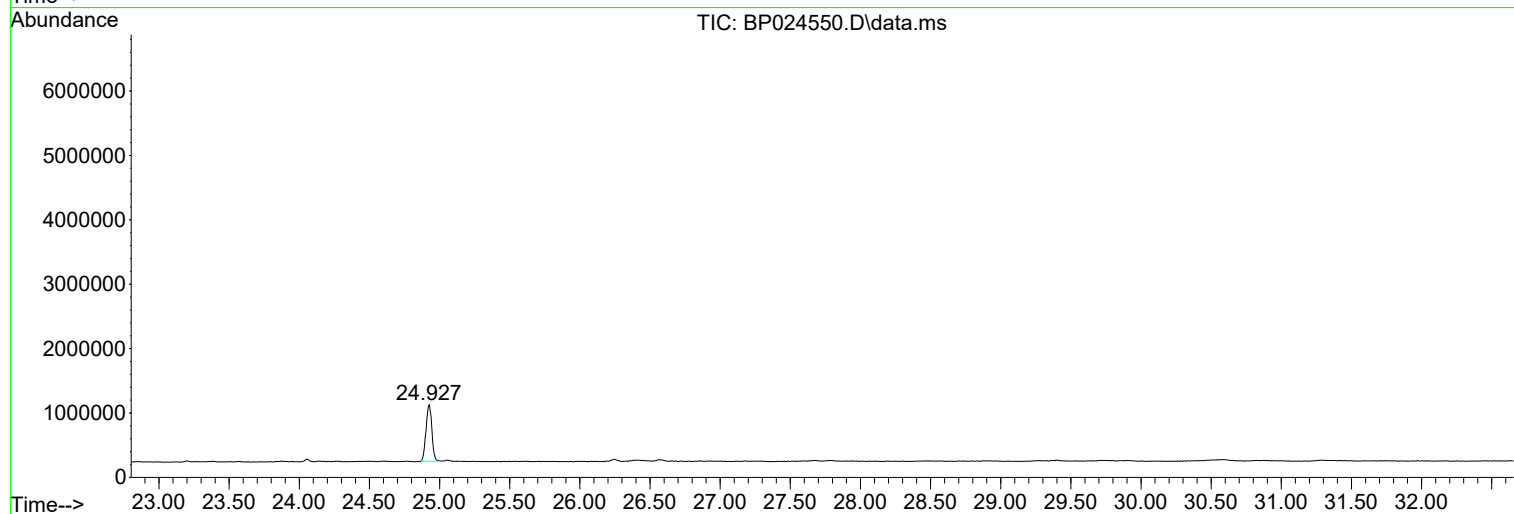
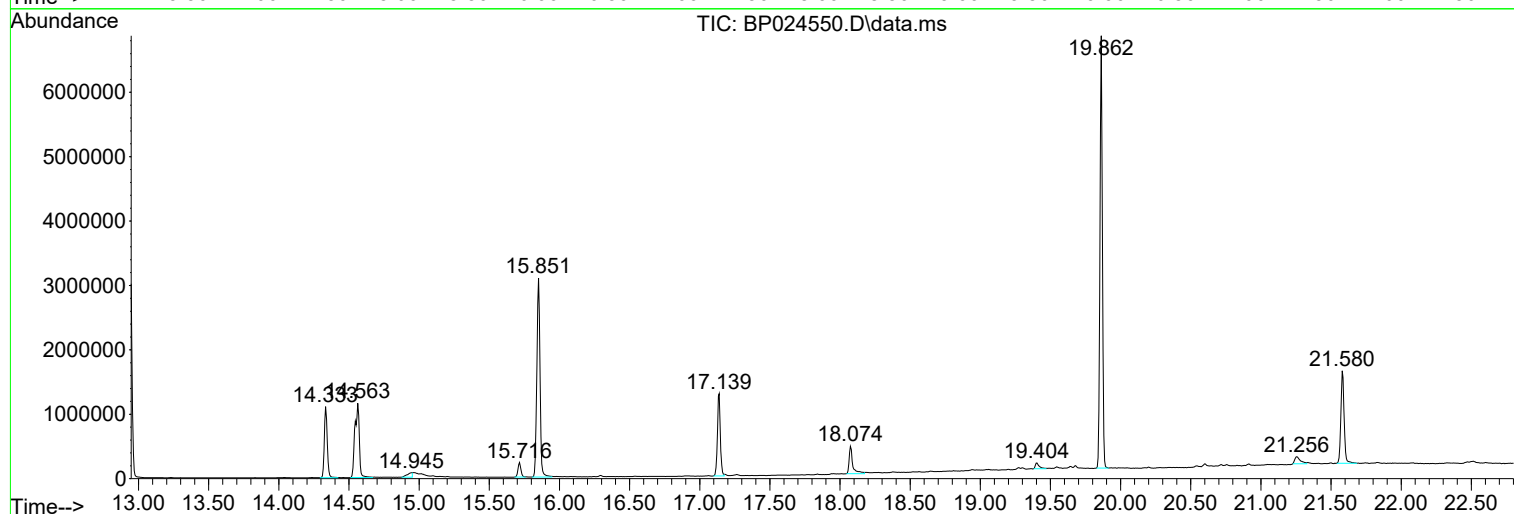
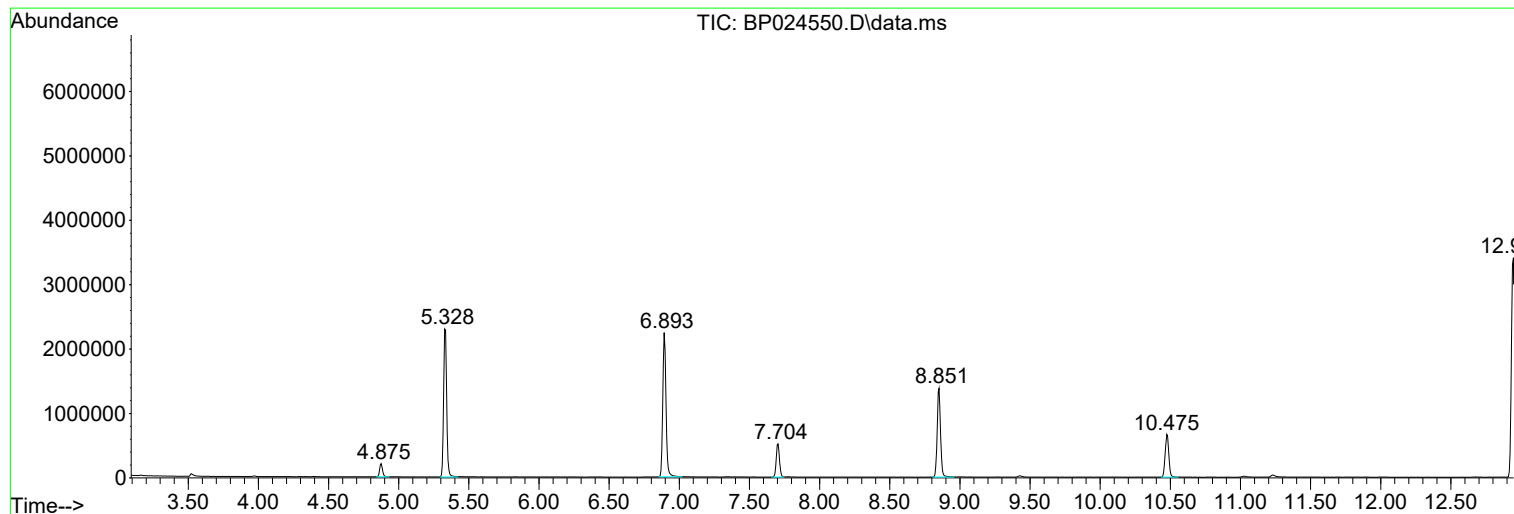
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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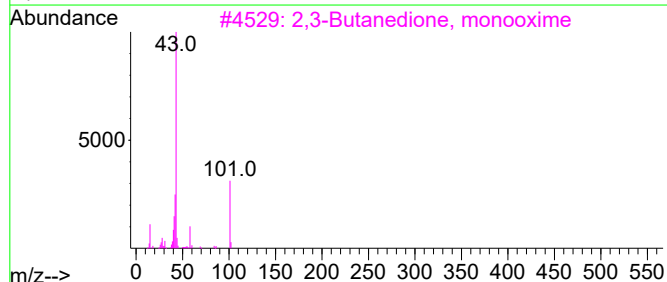
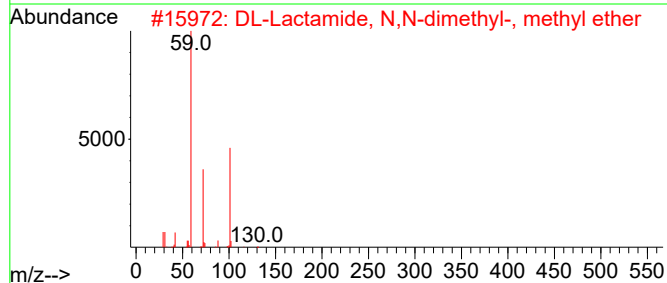
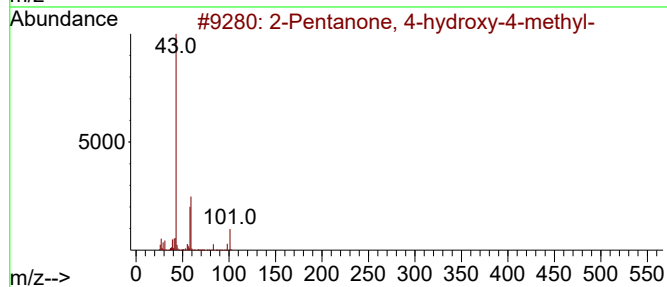
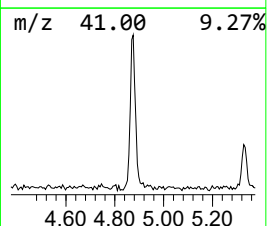
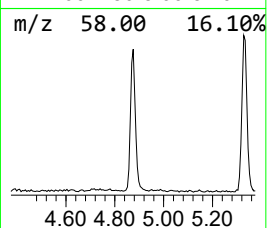
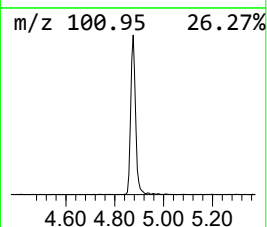
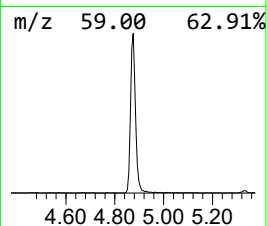
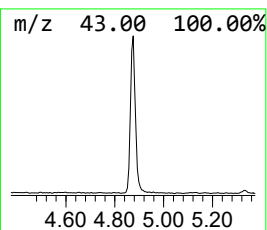
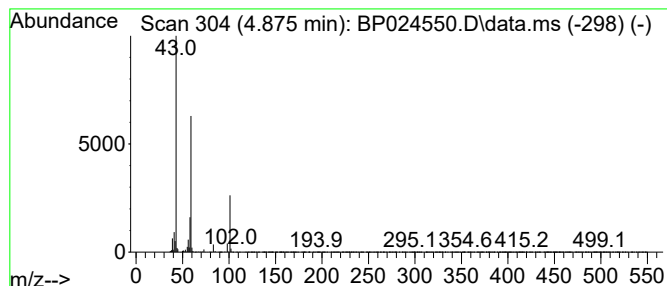
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	6.94 ng	292378	1,4-Dichlorobenzene-d4	7.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	38		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23		
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23		



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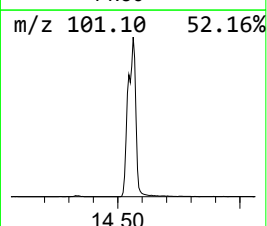
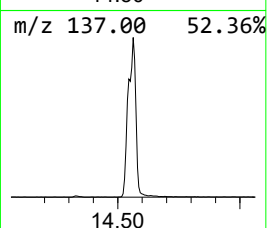
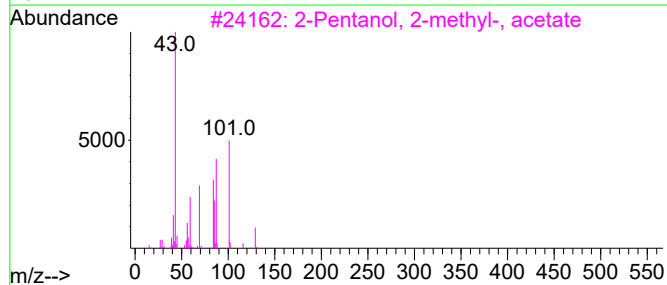
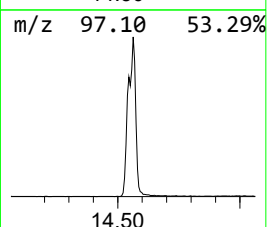
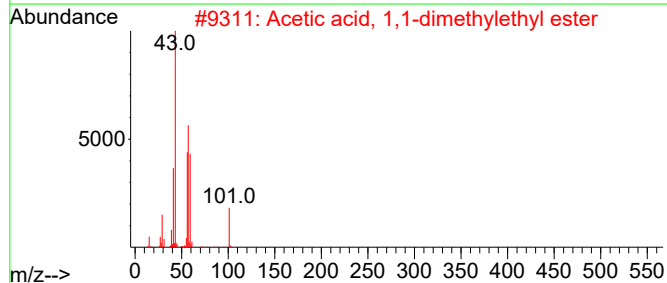
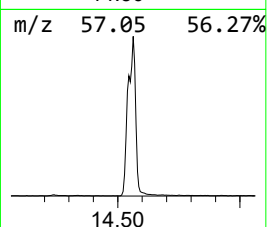
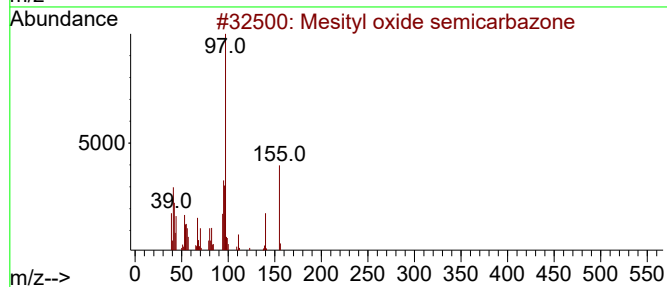
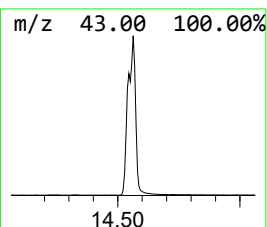
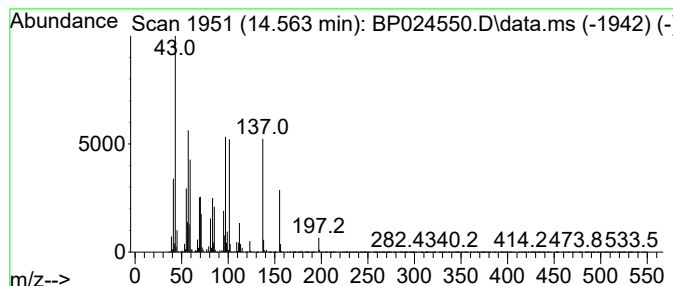
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown14.563 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	31.85 ng	2513160	Acenaphthene-d10	14.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesityl oxide semicarbazone	155	C7H13N3O	003780-62-9	22
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
3			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	14
5			2-Amino-5-fluorobenzoic acid	155	C7H6FN02	000446-08-2	11



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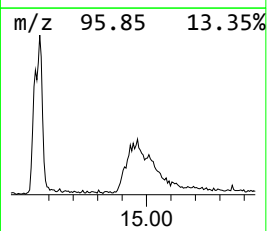
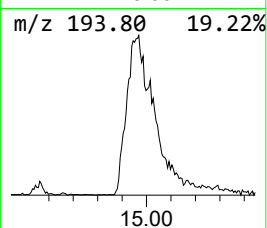
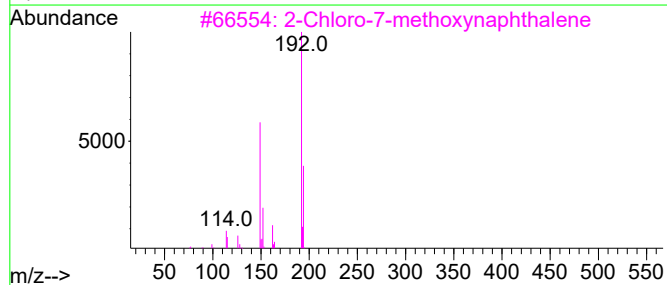
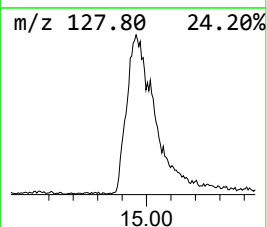
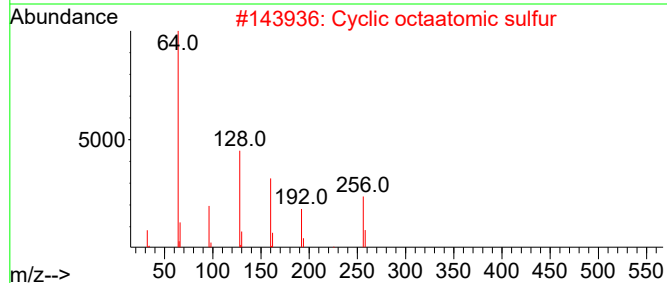
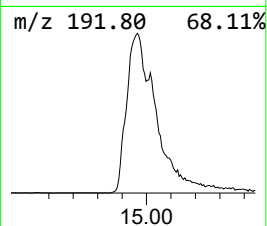
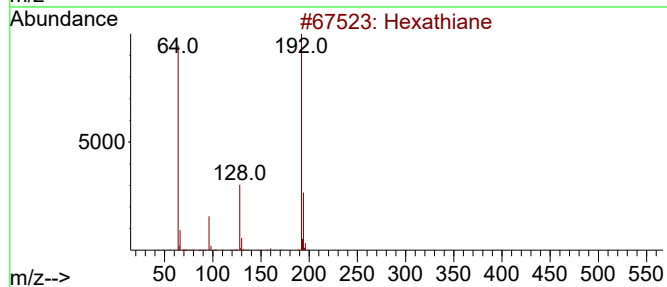
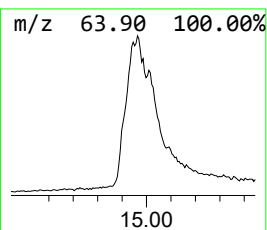
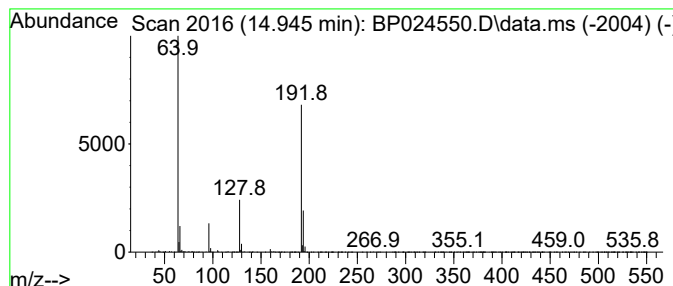
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Peak Number 3 Hexathiane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.945	2.28 ng	179533	Acenaphthene-d10	14.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	94
2			Cyclic octaatomic sulfur	256	S8	010544-50-0	9
3			2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	7
4			Cyclobutane, 1,1'-(1,1,2,2-tetra...	354	C10H6F12	035207-94-4	5
5			Sulfur dioxide	64	O2S	007446-09-5	4



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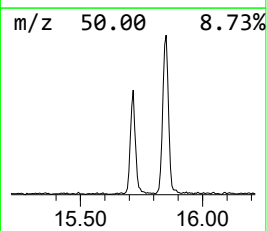
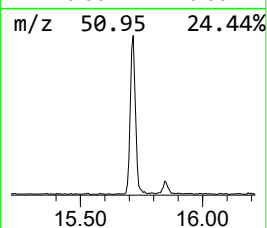
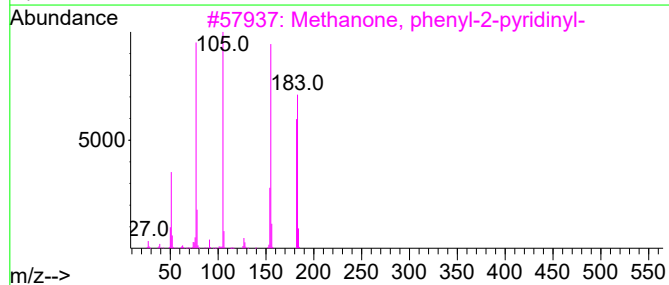
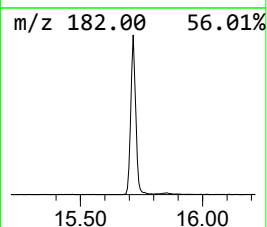
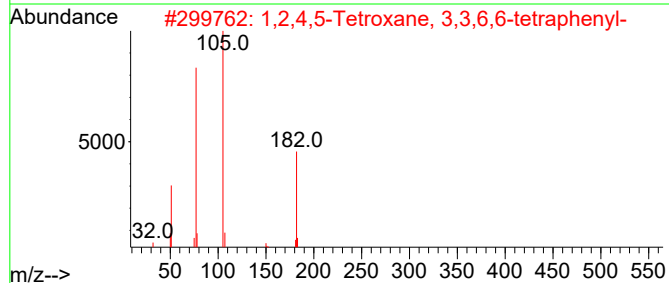
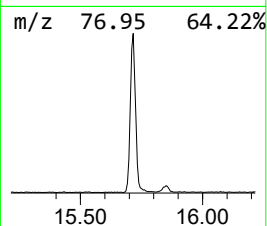
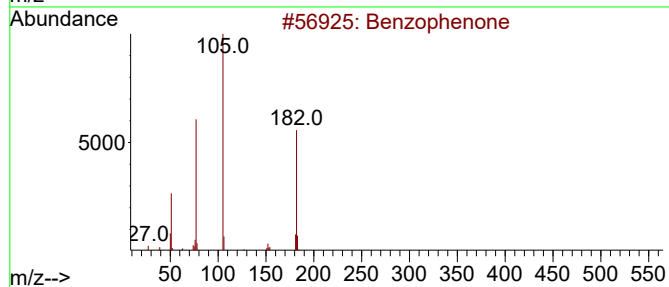
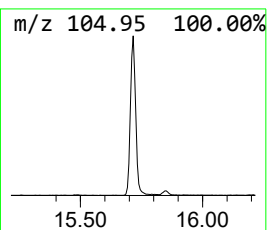
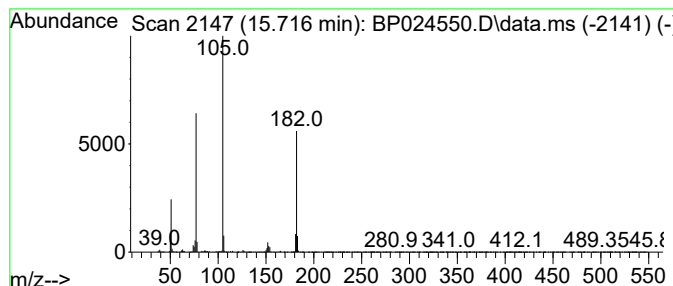
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.716	4.26 ng	336354	Acenaphthene-d10	14.333

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			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
4			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50
5			Azobenzene	182	C12H10N2	000103-33-3	45



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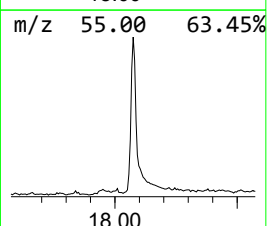
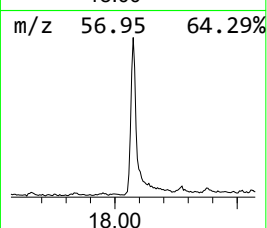
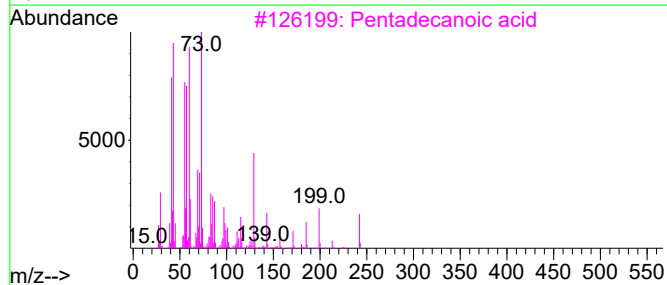
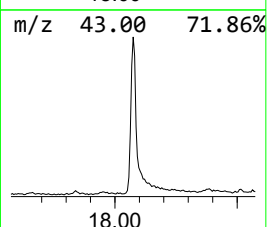
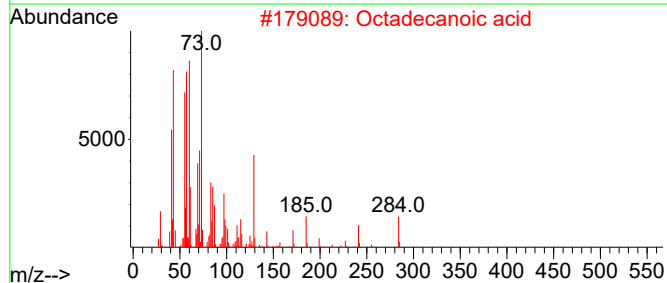
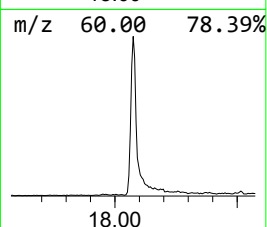
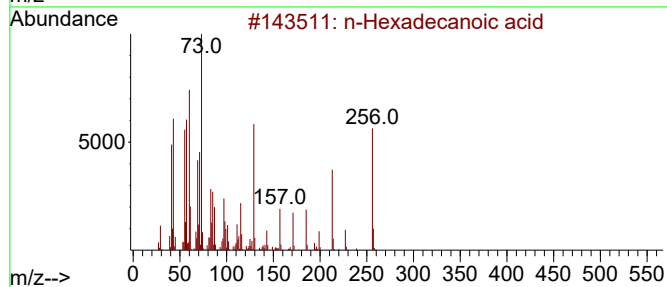
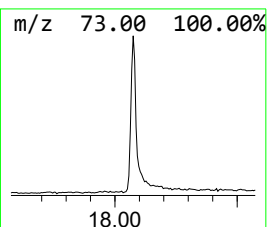
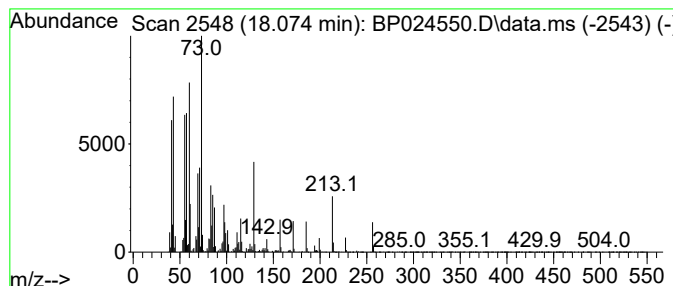
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	8.13 ng	755934	Phenanthrene-d10	17.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			Tridecanoic acid	214	C13H26O2	000638-53-9	87



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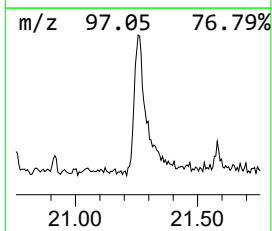
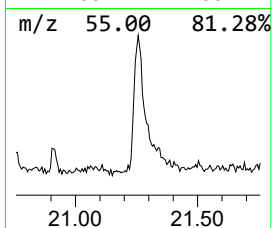
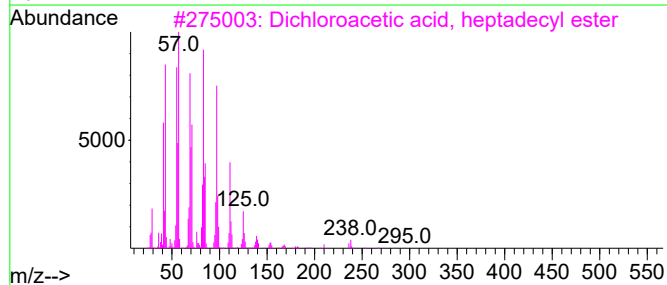
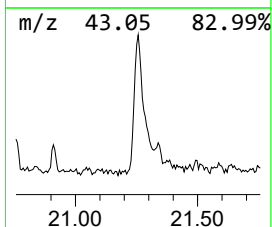
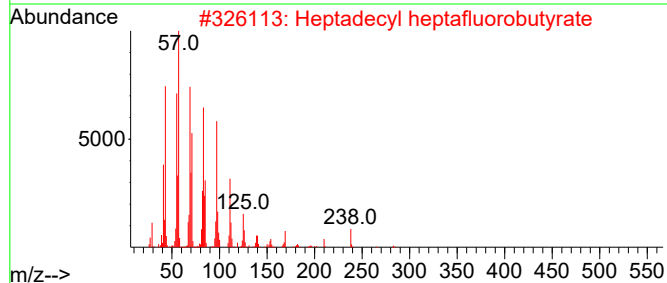
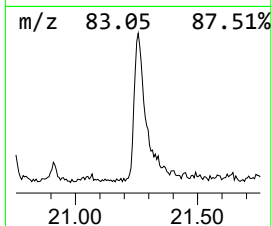
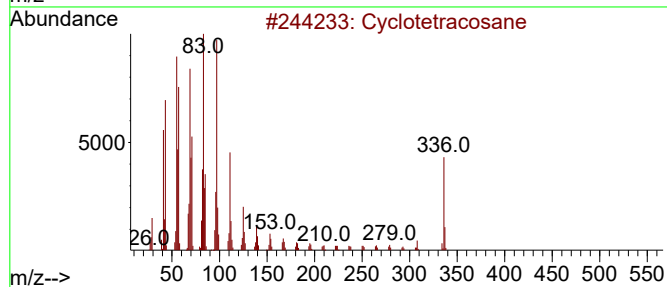
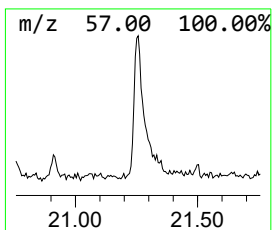
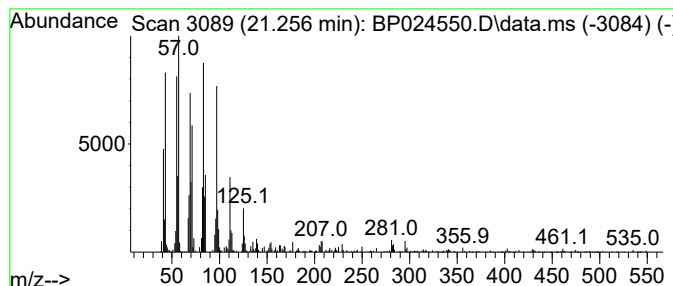
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.256	2.64 ng	304021	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	96
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP050625\
Data File : BP024550.D
Acq On : 06 May 2025 17:08
Operator : RC/JU
Sample : Q1956-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB2-4-5

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.875	6.9	ng	292378	1	7.704	842897	20.0
unknown14.563	14.563	31.9	ng	2513160	3	14.333	1578280	20.0
Hexathiane	14.945	2.3	ng	179533	3	14.333	1578280	20.0
Benzophenone	15.716	4.3	ng	336354	3	14.333	1578280	20.0
n-Hexadecanoic ...	18.074	8.1	ng	755934	4	17.139	1859390	20.0
Cyclotetracosane	21.256	2.6	ng	304021	5	21.580	2306730	20.0