

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
 Data File : BP013852.D
 Acq On : 17 Feb 2023 19:07
 Operator : CG/JU
 Sample : 01586-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-3

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-BP021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013852.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.175	329	338	347	rBV	893151	1238780	20.75%	3.507%
2	5.646	412	418	424	rBV	153271	221619	3.71%	0.627%
3	7.257	684	692	706	rBV	885470	1457573	24.42%	4.126%
4	8.110	826	837	843	rBV	575119	937636	15.71%	2.654%
5	9.281	1028	1036	1050	rBV	808781	1376181	23.05%	3.896%
6	10.934	1310	1317	1323	rBV	703739	1186982	19.88%	3.360%
7	13.369	1723	1731	1743	rBV	2327851	3430727	57.47%	9.712%
8	14.745	1953	1965	1971	rBV	1192993	1771989	29.68%	5.016%
9	14.804	1971	1975	1982	rVB	46119	74871	1.25%	0.212%
10	16.098	2189	2195	2202	rVB	143107	212974	3.57%	0.603%
11	16.228	2213	2217	2226	rBV2	48335	70774	1.19%	0.200%
12	16.433	2248	2252	2254	rBV	44740	60138	1.01%	0.170%
13	16.457	2254	2256	2268	rVB5	43988	70138	1.17%	0.199%
14	17.233	2383	2388	2393	rBV3	68353	112515	1.88%	0.319%
15	17.498	2427	2433	2437	rBV	1565075	2286497	38.30%	6.473%
16	17.539	2437	2440	2449	rVV	452336	661433	11.08%	1.872%
17	17.633	2451	2456	2461	rVV	86261	132182	2.21%	0.374%
18	17.892	2497	2500	2508	rVB2	44933	63837	1.07%	0.181%
19	18.351	2573	2578	2582	rBV2	208531	290828	4.87%	0.823%
20	18.398	2583	2586	2594	rVB2	99612	148767	2.49%	0.421%
21	18.539	2605	2610	2614	rBV2	83728	158127	2.65%	0.448%
22	18.575	2614	2616	2622	rVB	56471	72332	1.21%	0.205%
23	18.633	2623	2626	2632	rBV2	48757	66840	1.12%	0.189%
24	19.239	2725	2729	2732	rBV2	82662	105587	1.77%	0.299%
25	19.369	2748	2751	2755	rBV2	44994	68661	1.15%	0.194%
26	19.492	2767	2772	2777	rVB	996949	1269772	21.27%	3.595%
27	19.574	2783	2786	2791	rVB2	79184	100274	1.68%	0.284%
28	19.810	2821	2826	2828	rBV3	159610	286837	4.81%	0.812%
29	19.845	2828	2832	2839	rVB	861473	1222259	20.48%	3.460%
30	20.027	2858	2863	2868	rBV	4764625	5969397	100.00%	16.899%
31	20.316	2908	2912	2916	rVB2	191633	286475	4.80%	0.811%
32	20.792	2991	2993	2997	rVB	113154	100086	1.68%	0.283%
33	21.245	3067	3070	3075	rBV2	436922	572984	9.60%	1.622%
34	21.574	3119	3126	3130	rBV2	2236504	3648114	61.11%	10.328%
35	21.616	3130	3133	3139	rVB	470202	615981	10.32%	1.744%
36	21.692	3142	3146	3152	rBV	1571900	2362197	39.57%	6.687%

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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-BP021623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.133	3555	3561	3567	rVB2	1322499	2611477	43.75%	7.393%
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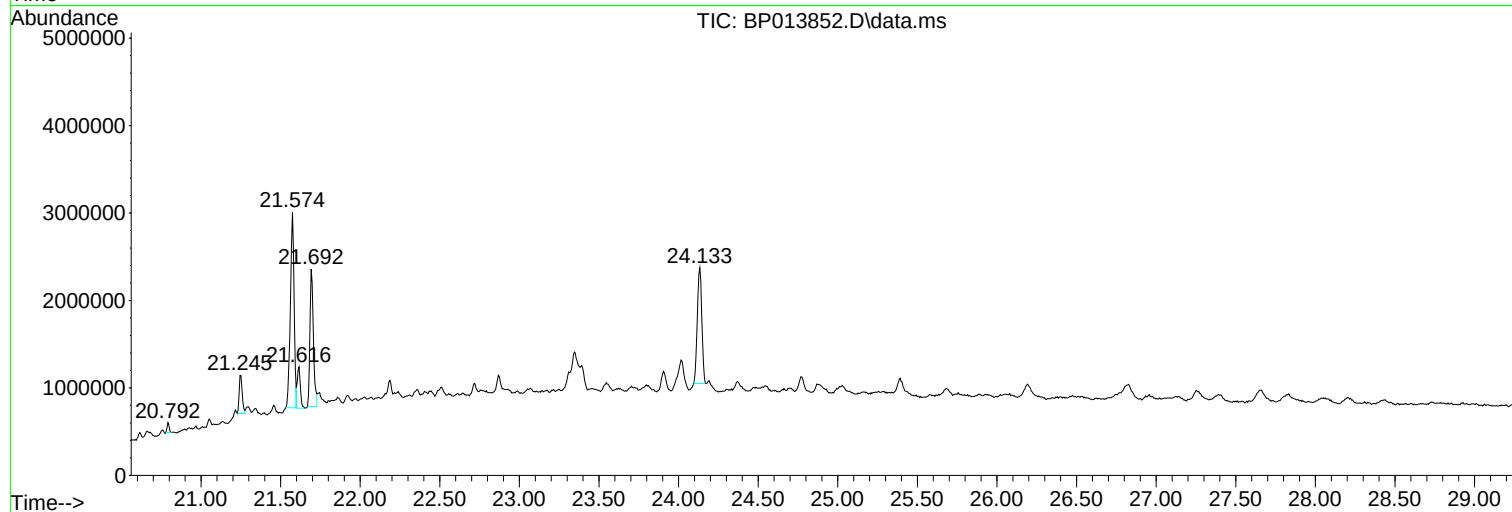
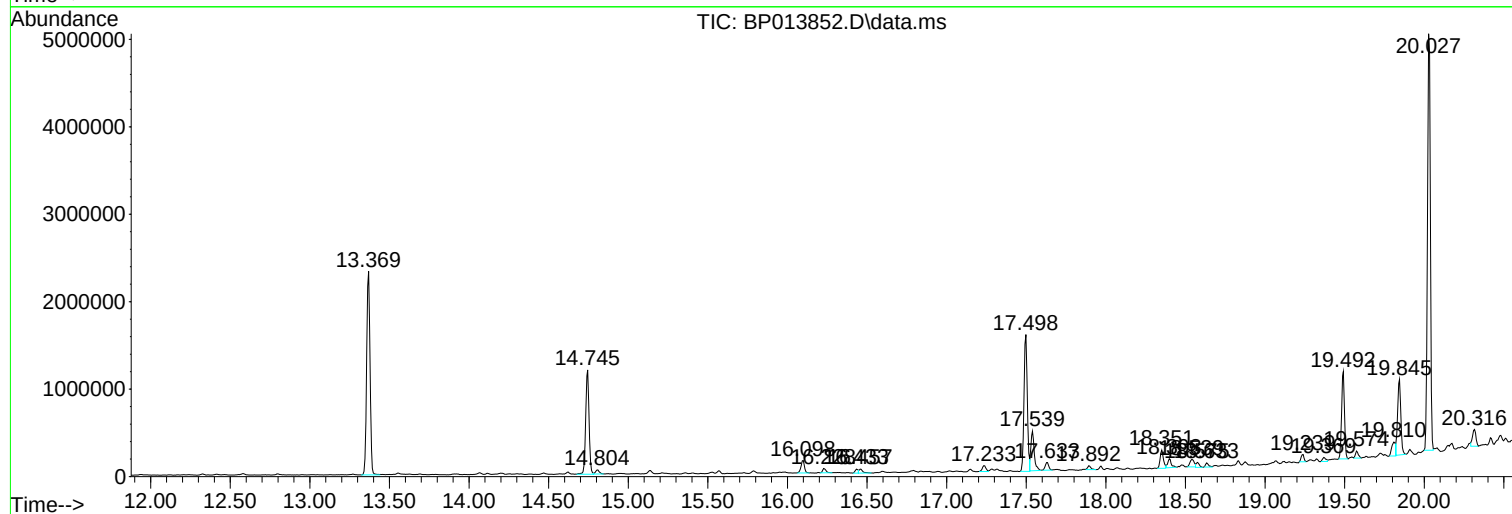
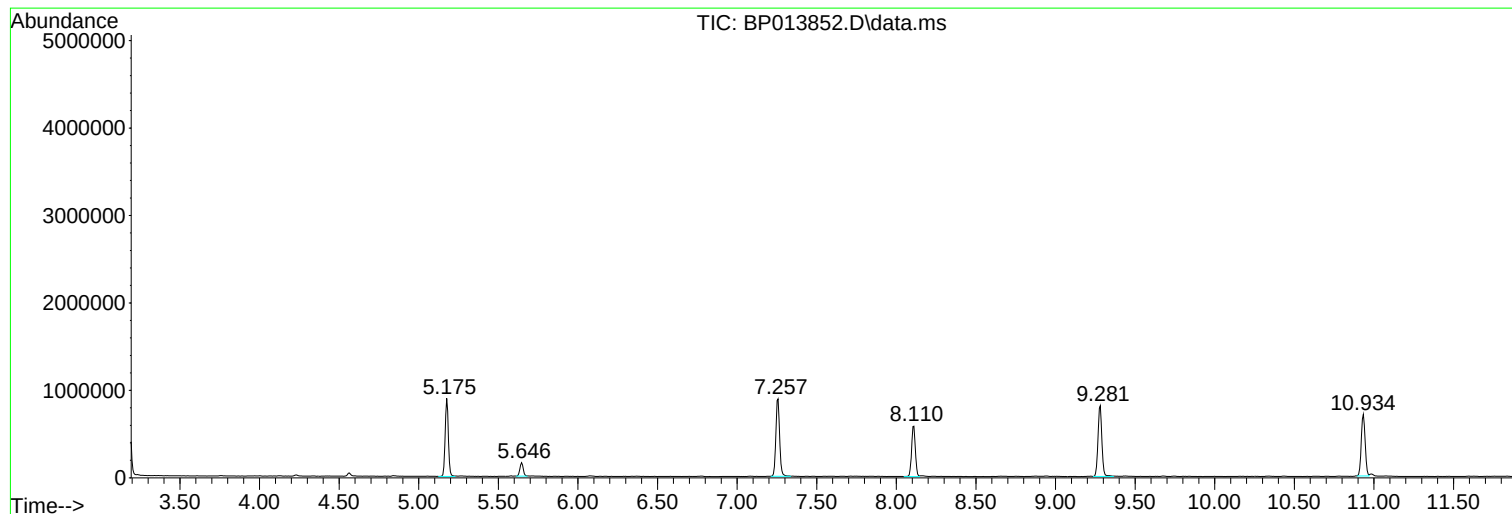
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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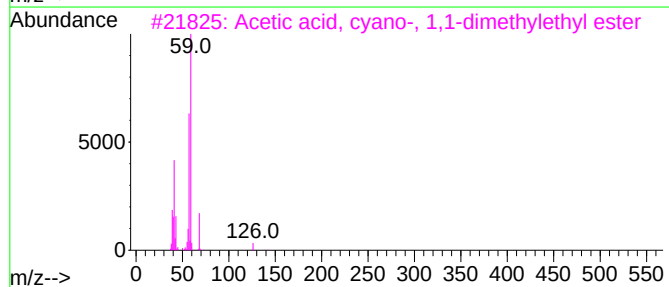
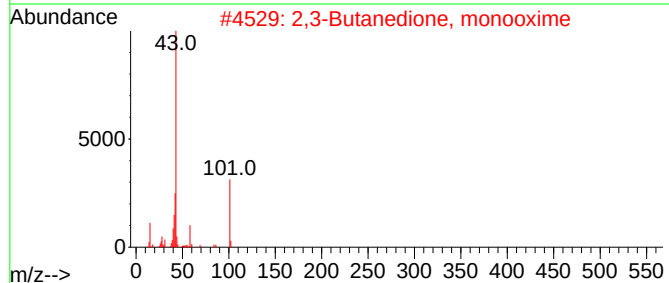
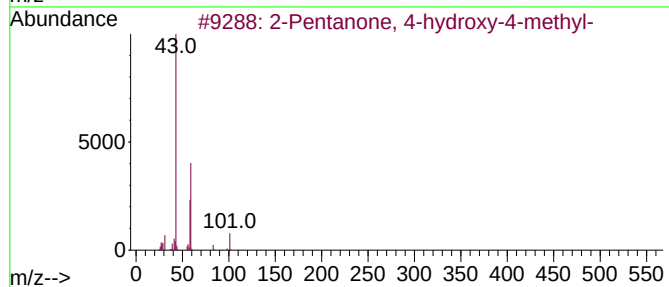
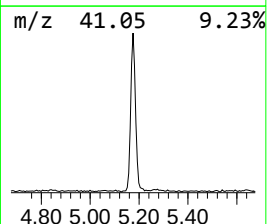
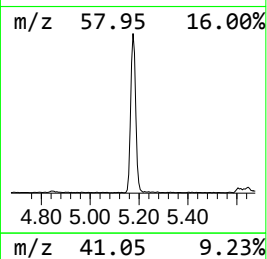
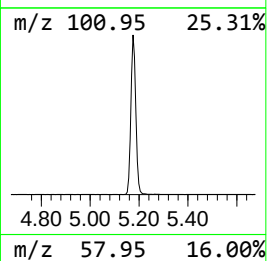
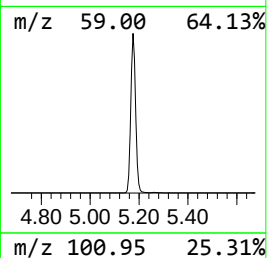
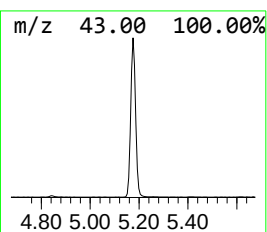
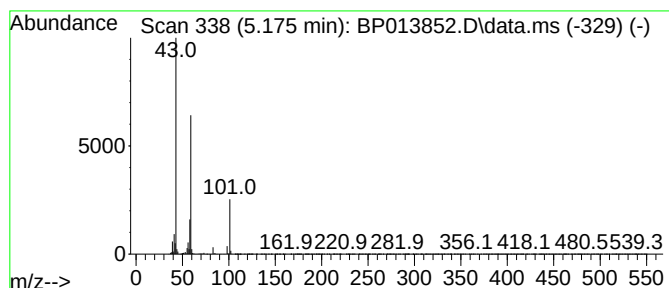
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	26.42 ng	1238780	1,4-Dichlorobenzene-d4	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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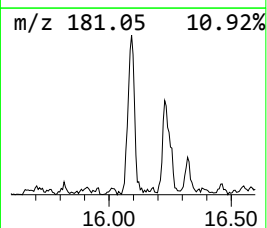
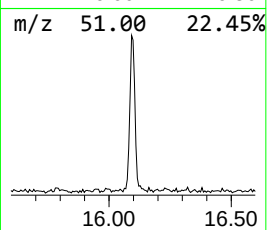
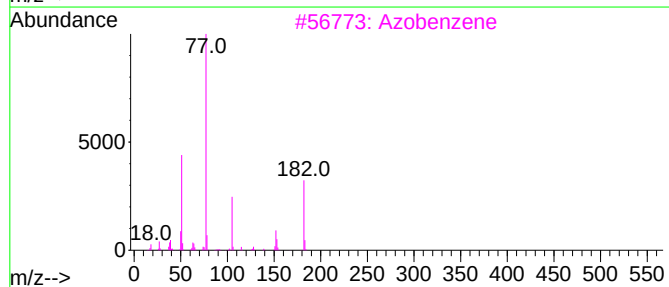
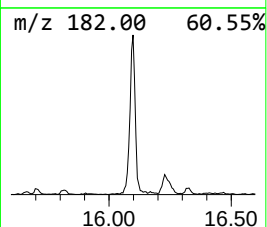
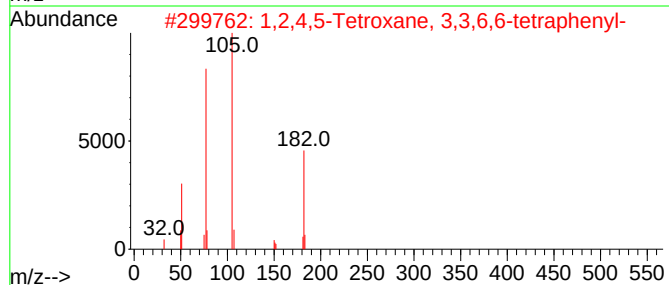
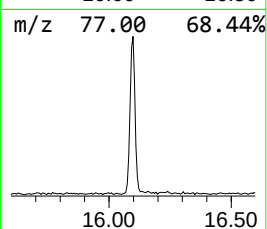
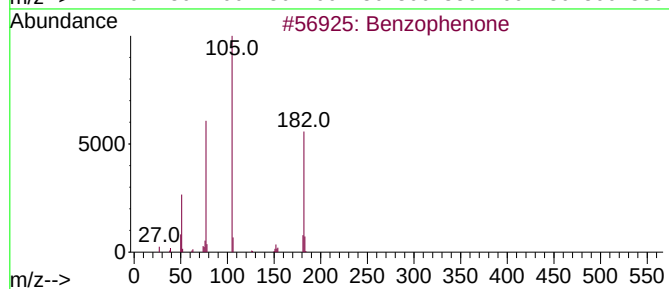
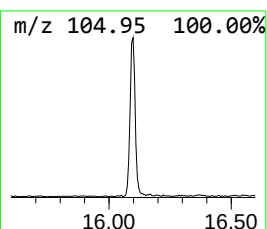
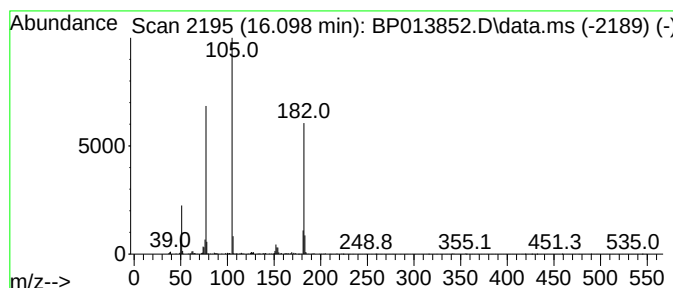
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	2.40 ng	212974	Acenaphthene-d10	14.745

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			Azobenzene	182	C12H10N2	000103-33-3	64
4			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50
5			1,2,4-Triazolo[4,3-b]pyridazine,...	182	C7H7ClN4	028593-26-2	38



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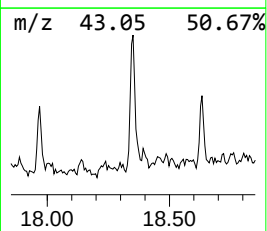
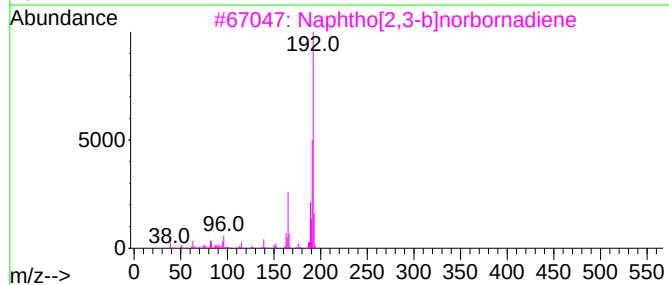
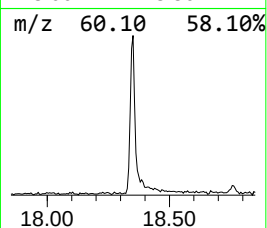
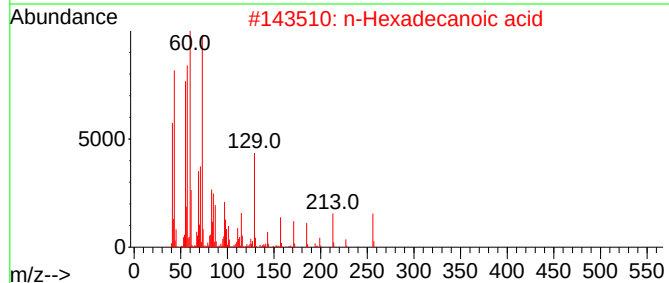
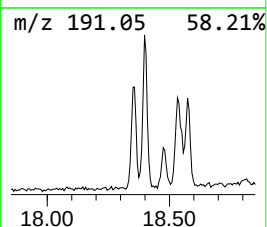
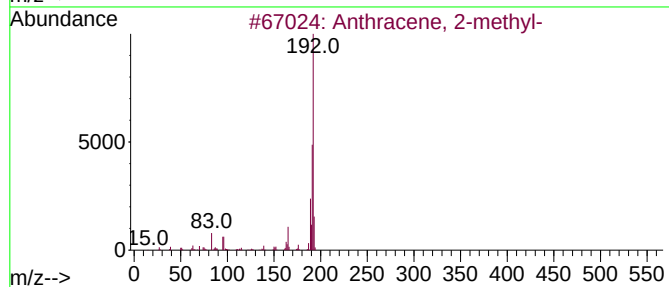
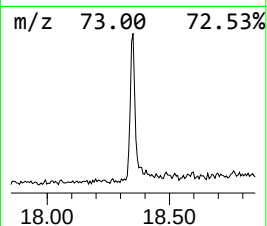
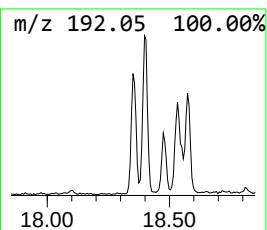
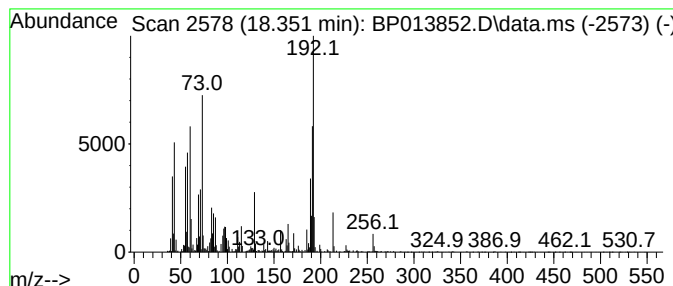
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	2.54 ng	290828	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	91
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
5			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90



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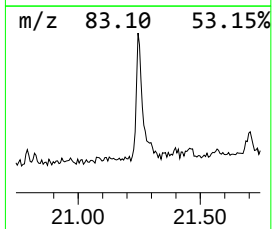
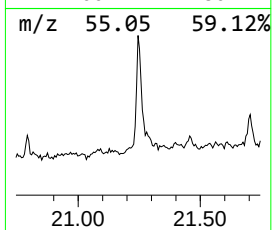
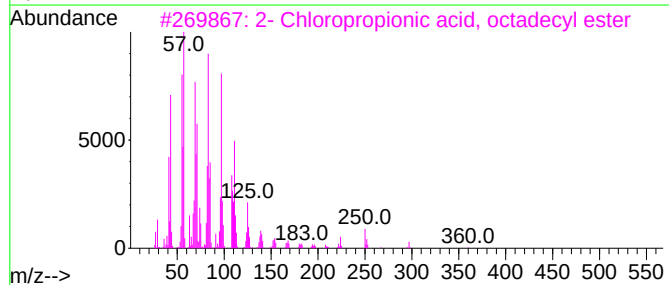
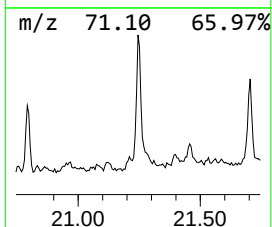
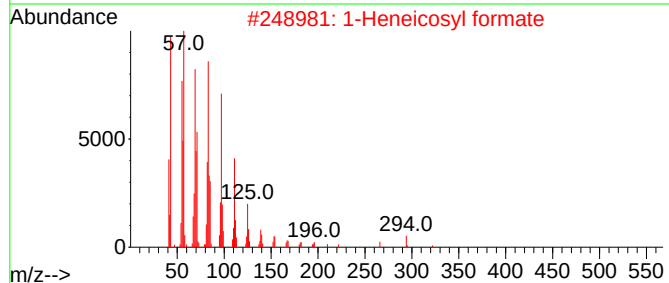
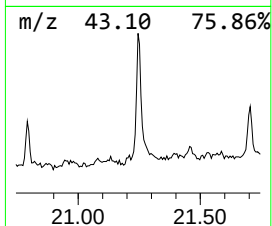
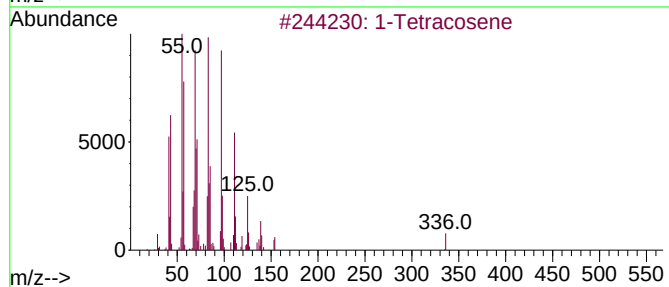
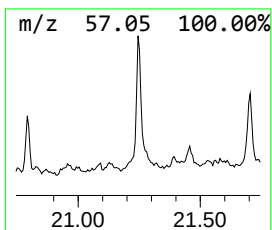
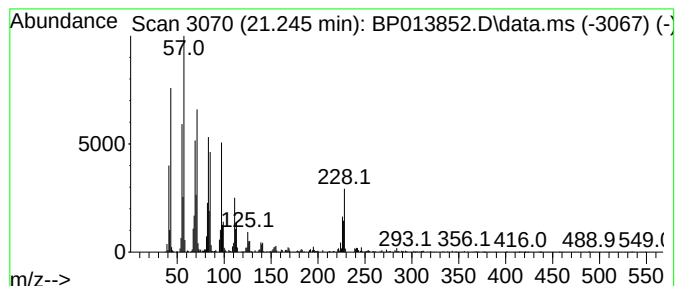
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	3.14 ng	572984	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	95
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4			Ether, 1-hexadecenyl methyl, (Z)-	254	C17H34O	020246-43-9	90
5			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87



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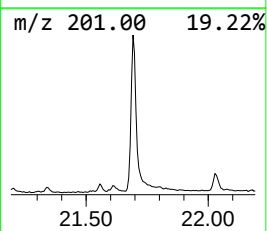
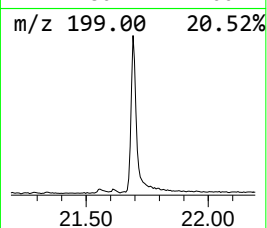
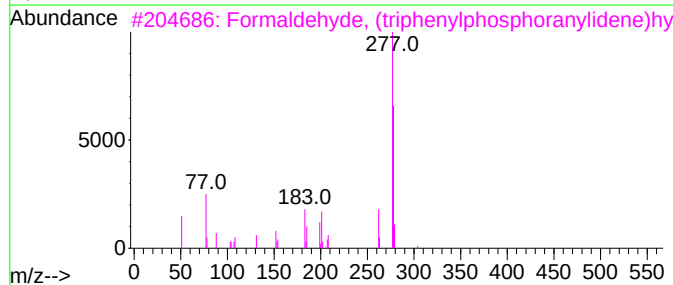
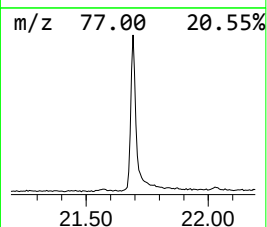
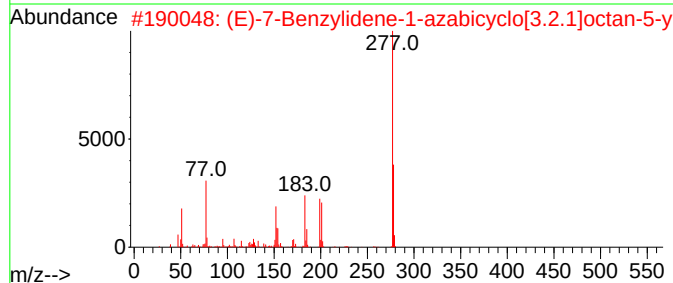
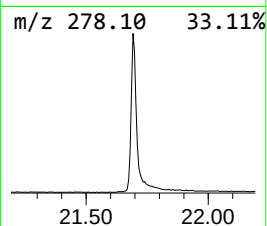
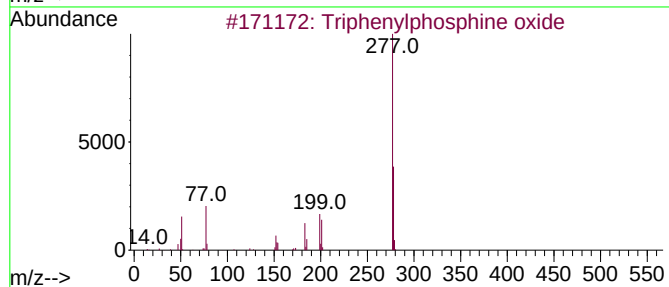
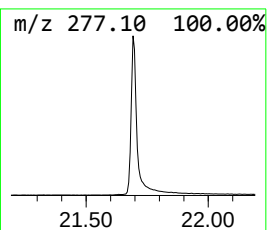
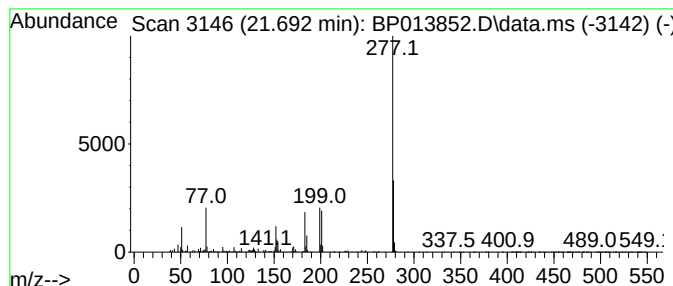
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.692	12.95 ng	2362200	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013852.D
Acq On : 17 Feb 2023 19:07
Operator : CG/JU
Sample : 01586-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.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-...	5.175	26.4	ng	1238780	1	8.110	937636	20.0
Benzophenone	16.098	2.4	ng	212974	3	14.745	1771990	20.0
Anthracene, 2-m...	18.351	2.5	ng	290828	4	17.498	2286500	20.0
1-Tetracosene	21.245	3.1	ng	572984	5	21.574	3648110	20.0
Triphenylphosph...	21.692	12.9	ng	2362200	5	21.574	3648110	20.0