

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
 Data File : BP013855.D
 Acq On : 17 Feb 2023 20:50
 Operator : CG/JU
 Sample : 01586-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-2

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: BP013855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.940	123	128	134	rBV	77115	98446	1.65%	0.215%
2	4.564	228	234	249	rBV	4165502	5742027	96.50%	12.537%
3	5.187	331	340	352	rBV	3307211	4960171	83.36%	10.830%
4	5.646	413	418	425	rBV	58377	91753	1.54%	0.200%
5	7.258	683	692	709	rBV	828509	1362036	22.89%	2.974%
6	8.110	825	837	844	rBV	638882	1016251	17.08%	2.219%
7	8.769	942	949	958	rBV	44871	80476	1.35%	0.176%
8	9.281	1029	1036	1051	rBV	1031480	1700366	28.58%	3.712%
9	10.934	1311	1317	1324	rBV	832831	1391924	23.39%	3.039%
10	13.369	1723	1731	1742	rBV	2826761	4126744	69.35%	9.010%
11	14.745	1955	1965	1972	rBV	1336690	1986758	33.39%	4.338%
12	14.810	1972	1976	1981	rVB	53563	83708	1.41%	0.183%
13	15.139	2027	2032	2040	rVB2	42769	67072	1.13%	0.146%
14	16.098	2190	2195	2203	rVB	259527	355182	5.97%	0.775%
15	16.439	2248	2253	2255	rBV2	52648	85821	1.44%	0.187%
16	17.233	2385	2388	2393	rBV4	68947	90473	1.52%	0.198%
17	17.498	2427	2433	2437	rBV	1710518	2451251	41.19%	5.352%
18	17.545	2437	2441	2448	rVV	569247	873559	14.68%	1.907%
19	17.633	2452	2456	2460	rVB	132257	182426	3.07%	0.398%
20	17.898	2497	2501	2509	rVB	54587	88818	1.49%	0.194%
21	18.351	2574	2578	2583	rBV2	176543	274661	4.62%	0.600%
22	18.404	2583	2587	2594	rVB2	137530	197725	3.32%	0.432%
23	18.545	2606	2611	2614	rBV2	122391	217585	3.66%	0.475%
24	19.239	2726	2729	2734	rVB	113074	126672	2.13%	0.277%
25	19.492	2767	2772	2777	rBV	1275363	1647056	27.68%	3.596%
26	19.845	2828	2832	2840	rVB	1075443	1451354	24.39%	3.169%
27	20.033	2859	2864	2869	rBV	4992841	5950426	100.00%	12.992%
28	21.251	3068	3071	3076	rVB2	631334	731191	12.29%	1.596%
29	21.580	3121	3127	3131	rBV3	1945814	3312548	55.67%	7.232%
30	21.621	3131	3134	3140	rVB	530855	698202	11.73%	1.524%
31	21.698	3143	3147	3153	rBV	1326054	1909159	32.08%	4.168%
32	24.139	3558	3562	3570	rVB2	1219435	2449720	41.17%	5.349%

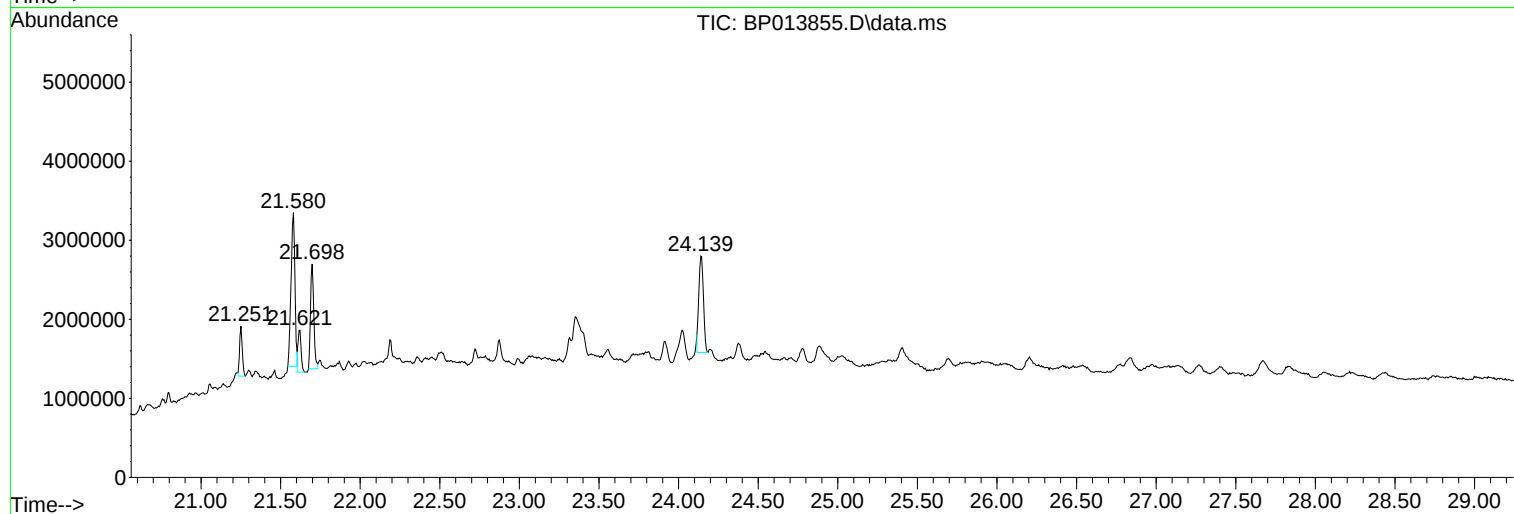
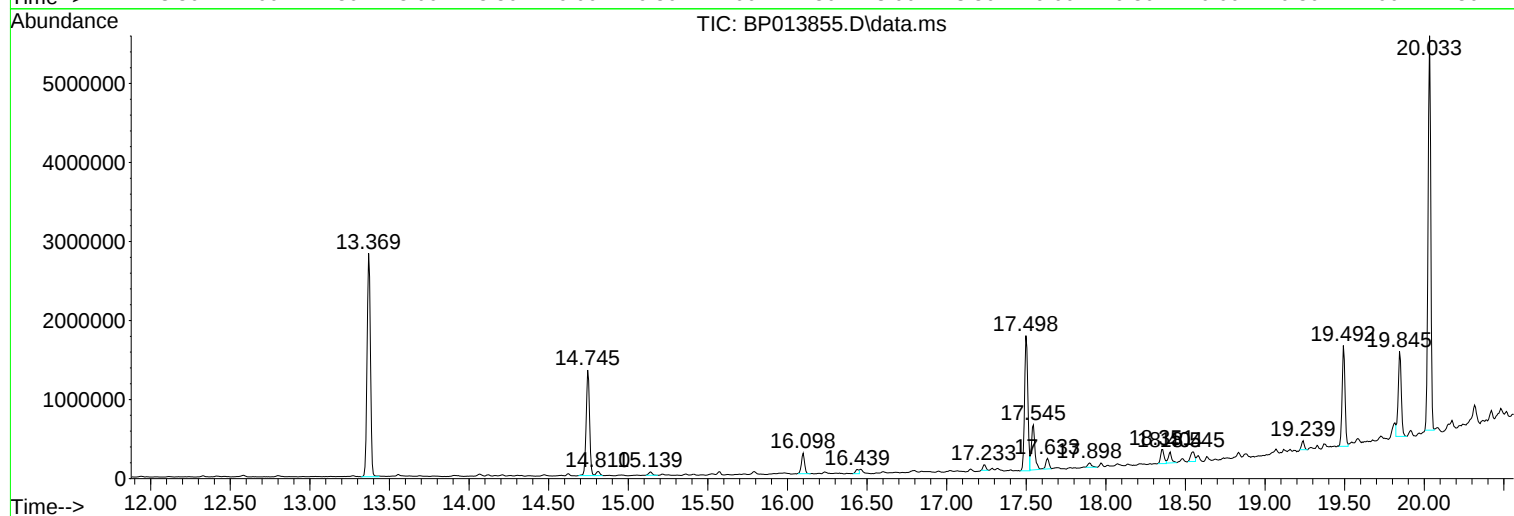
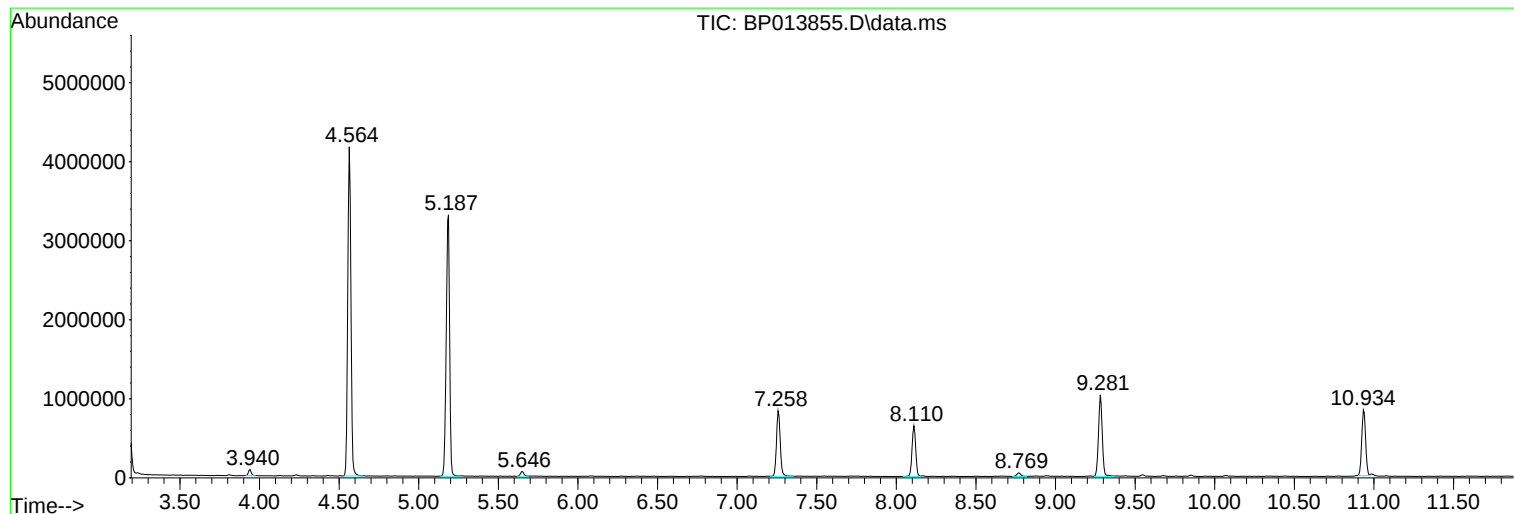
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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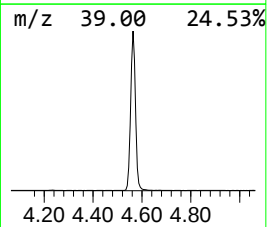
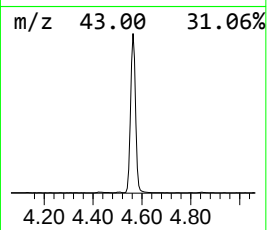
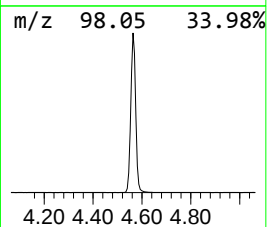
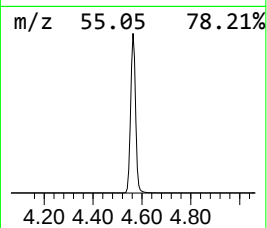
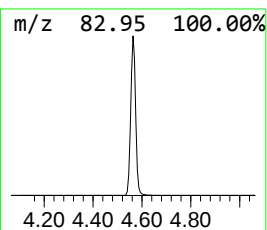
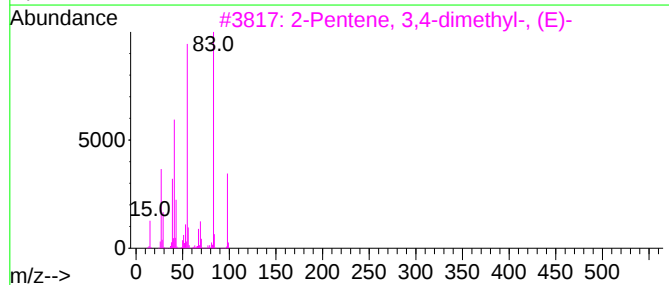
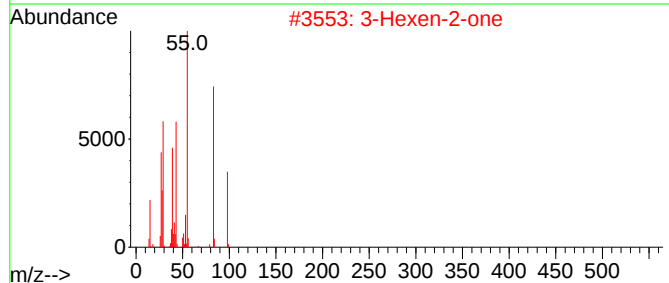
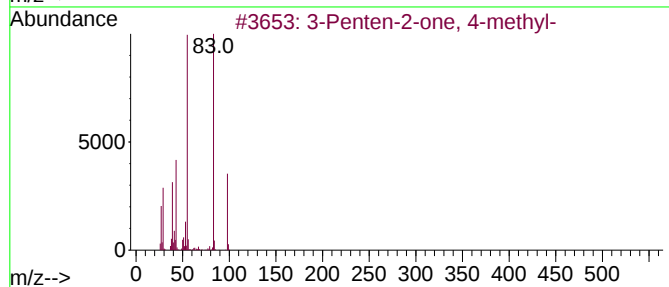
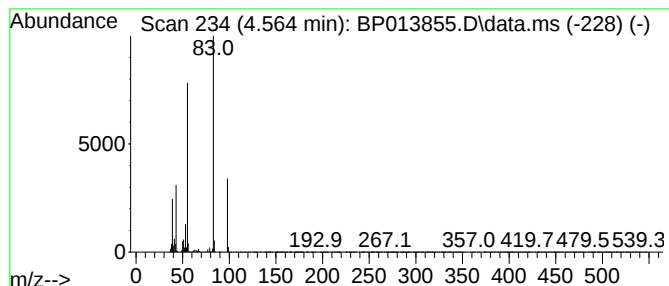
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.564	113.00 ng	5742030	1,4-Dichlorobenzene-d4	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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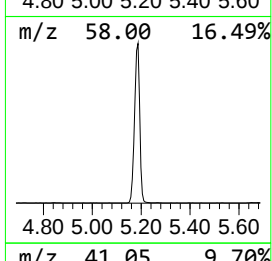
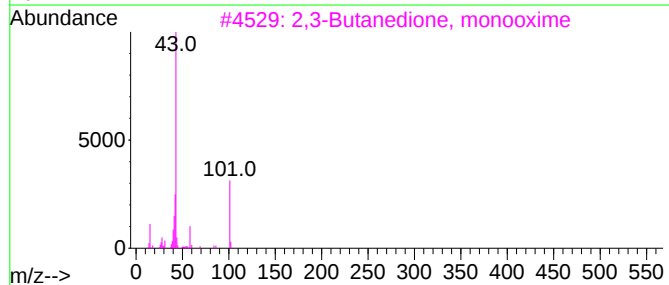
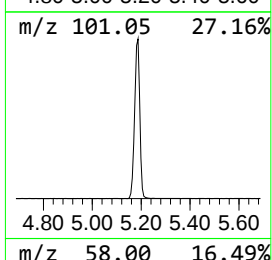
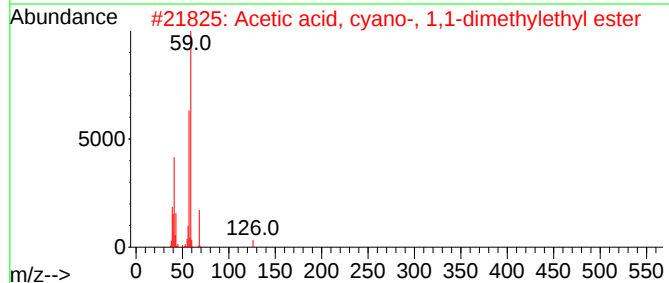
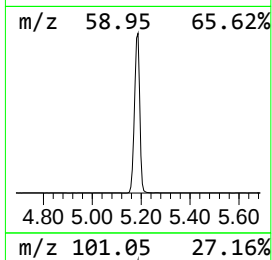
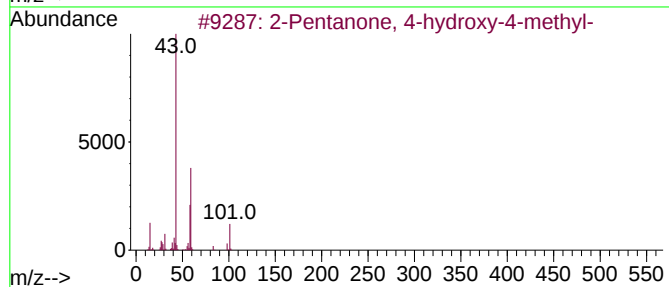
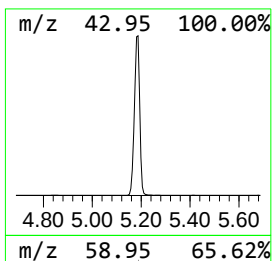
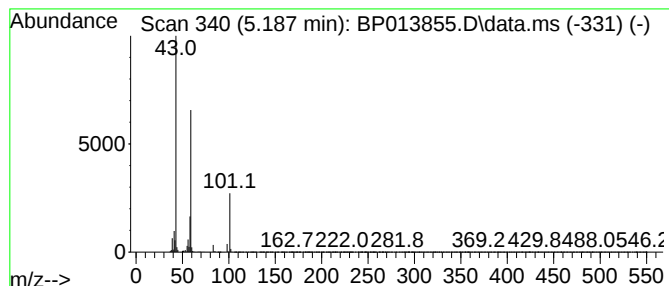
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	97.62 ng	4960170	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	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Acetone	58	C3H6O	000067-64-1	10



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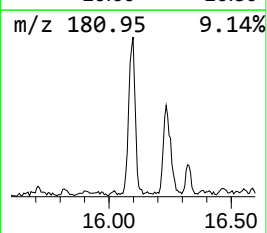
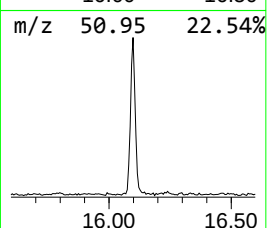
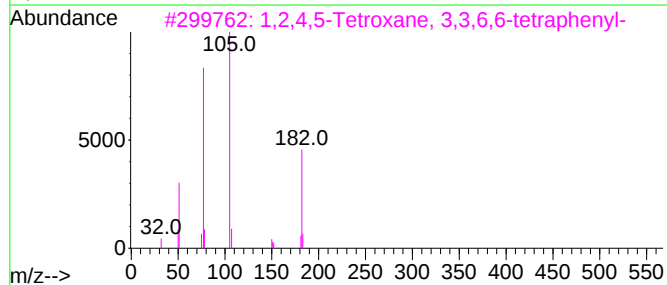
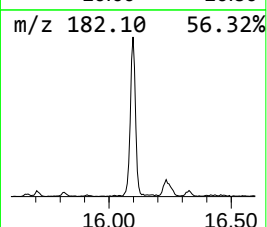
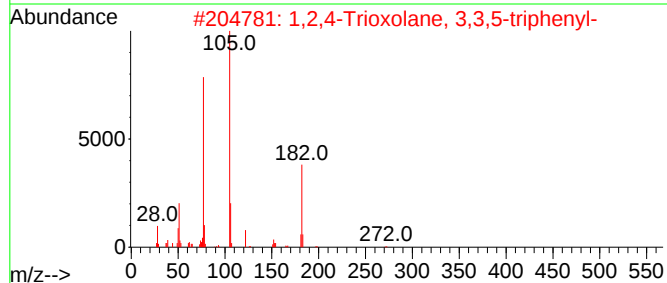
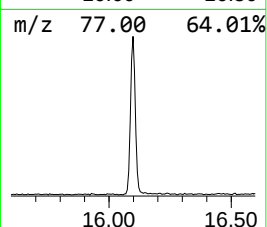
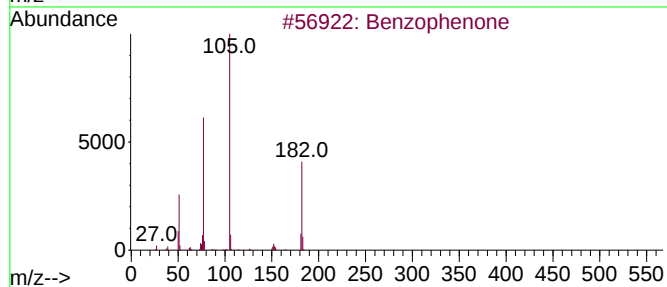
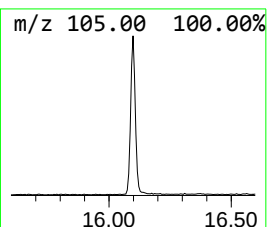
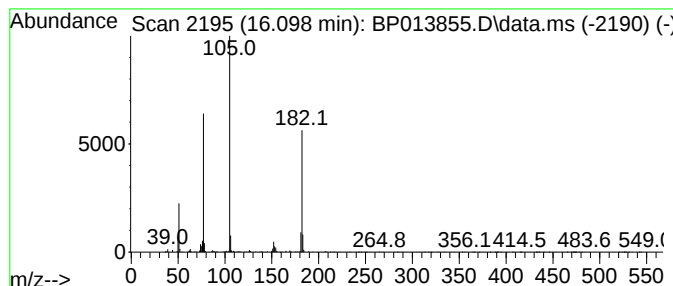
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	3.58 ng	355182	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-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	64
4			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	45
5			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	42



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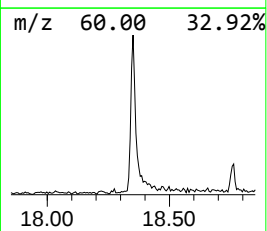
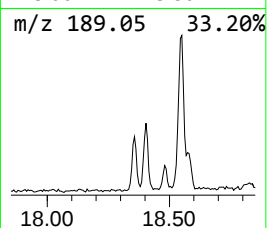
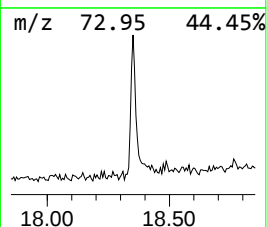
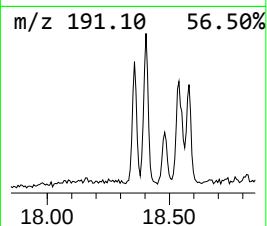
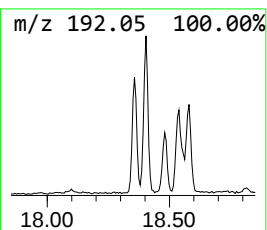
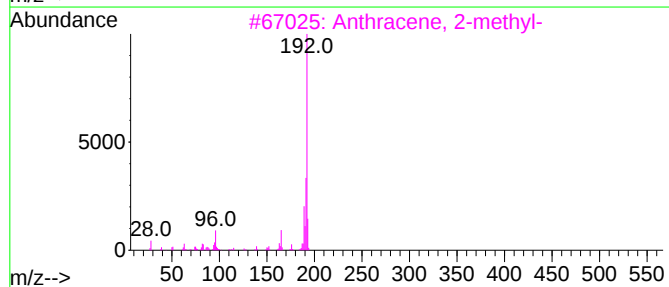
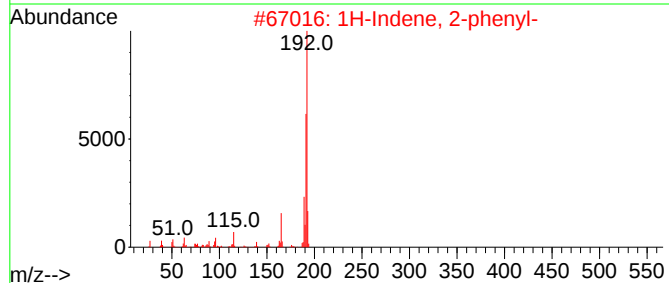
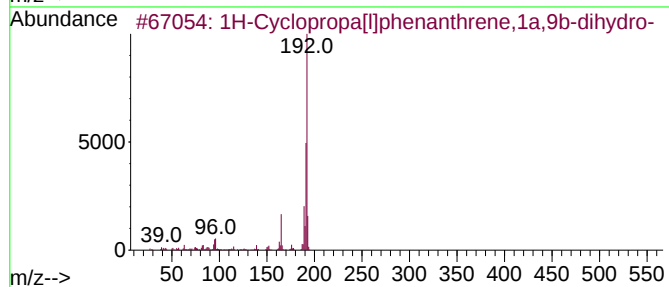
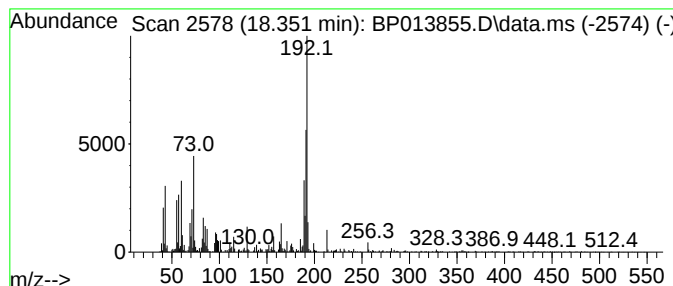
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1H-Cyclopropa[l]phenanthren... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	2.24 ng	274661	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
2			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	90
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90



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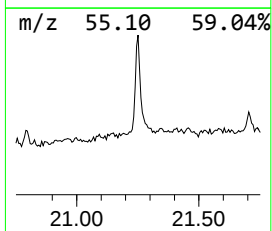
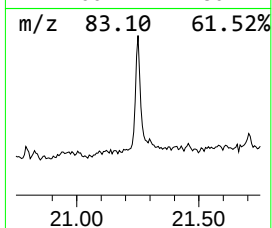
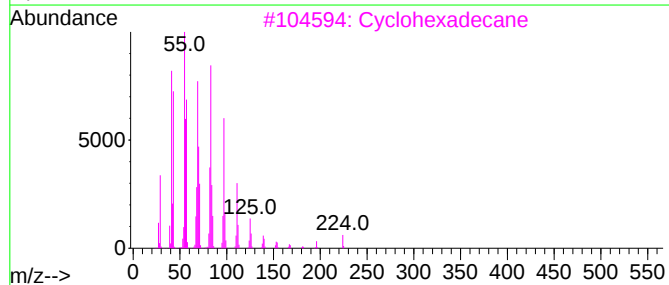
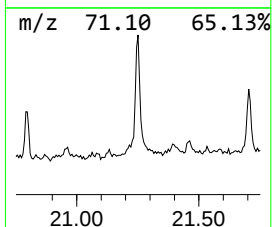
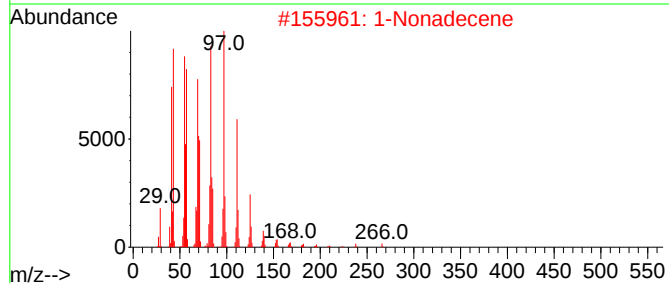
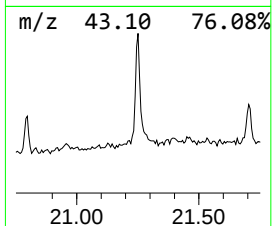
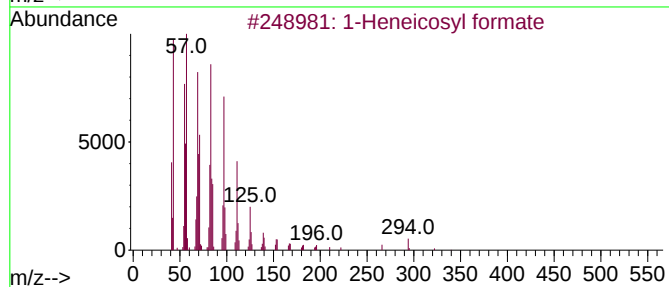
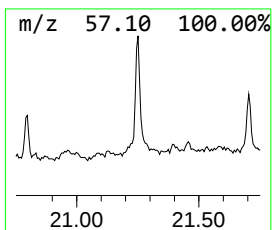
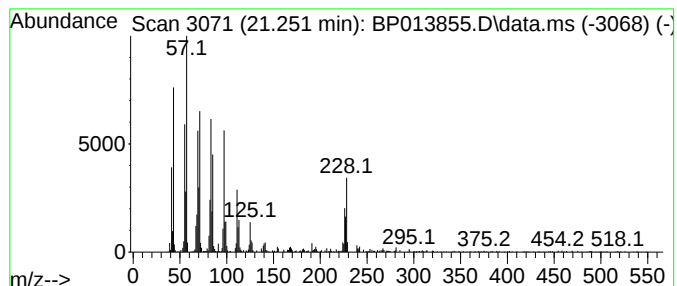
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Peak Number 5 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	4.41 ng	731191	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
2			1-Nonadecene	266	C19H38	018435-45-5	90
3			Cyclohexadecane	224	C16H32	000295-65-8	89
4			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	87



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COMP-2

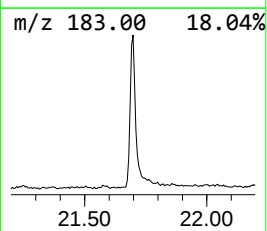
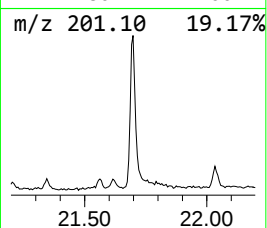
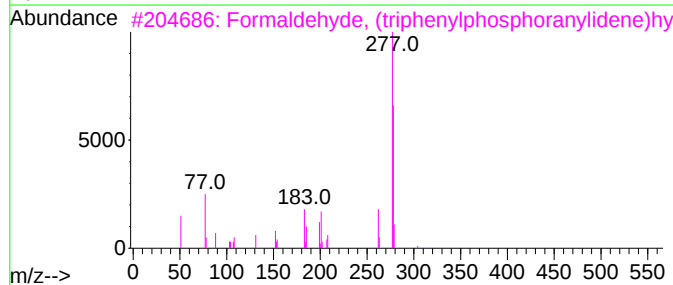
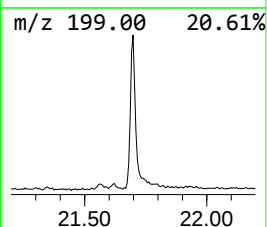
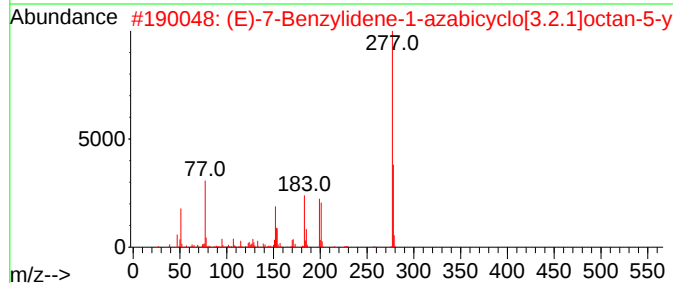
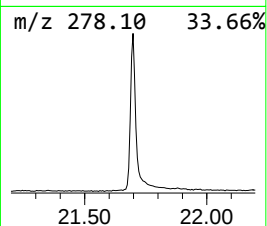
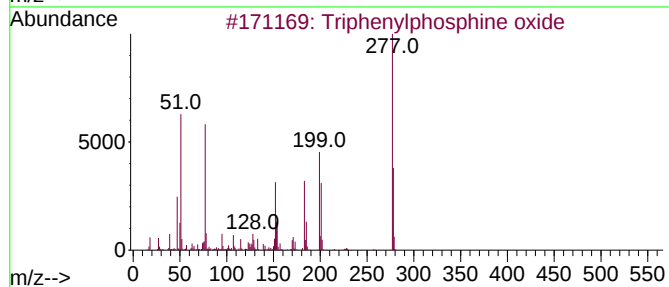
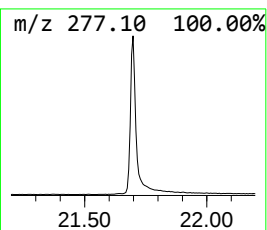
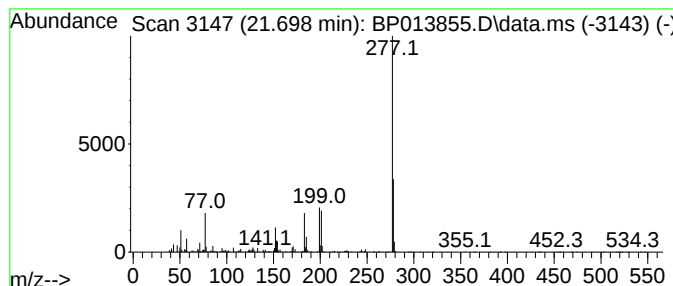
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.698	11.53 ng	1909160	Chrysene-d12	21.580

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	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	32
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25
5			[1,2,4]Triazolo[1,5-a]pyrimidine...	278	C15H14N6	1000350-69-0	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013855.D
Acq On : 17 Feb 2023 20:50
Operator : CG/JU
Sample : 01586-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-2

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
3-Penten-2-one,...	4.564	113.0	ng	5742030	1	8.110	1016250	20.0
2-Pentanone, 4-...	5.187	97.6	ng	4960170	1	8.110	1016250	20.0
Benzophenone	16.098	3.6	ng	355182	3	14.745	1986760	20.0
1H-Cyclopropa[l...	18.351	2.2	ng	274661	4	17.498	2451250	20.0
1-Heneicosyl fo...	21.251	4.4	ng	731191	5	21.580	3312550	20.0
Triphenylphosph...	21.698	11.5	ng	1909160	5	21.580	3312550	20.0