

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
 Data File : BP013853.D
 Acq On : 17 Feb 2023 19:41
 Operator : CG/JU
 Sample : 01586-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-4

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: BP013853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.564	228	234	248	rBV	2121899	2961745	45.15%	7.187%
2	5.181	330	339	350	rBV	3070929	4340518	66.17%	10.533%
3	5.646	413	418	426	rBV	96923	148196	2.26%	0.360%
4	7.257	684	692	708	rBV	1093480	1767865	26.95%	4.290%
5	8.110	829	837	843	rBV	517452	837979	12.77%	2.034%
6	9.281	1028	1036	1044	rBV	983541	1613136	24.59%	3.915%
7	10.934	1310	1317	1323	rBV	678217	1130780	17.24%	2.744%
8	13.369	1723	1731	1743	rBV	2449337	3617473	55.15%	8.779%
9	14.745	1959	1965	1972	rVV	1010826	1492520	22.75%	3.622%
10	14.810	1972	1976	1982	rVB	45648	70632	1.08%	0.171%
11	15.139	2026	2032	2037	rBV2	47834	79685	1.21%	0.193%
12	15.569	2101	2105	2110	rVB2	52878	68518	1.04%	0.166%
13	16.098	2189	2195	2202	rVB	209295	295388	4.50%	0.717%
14	16.433	2248	2252	2255	rBV	63753	101380	1.55%	0.246%
15	17.233	2384	2388	2393	rBV3	68638	94640	1.44%	0.230%
16	17.498	2427	2433	2437	rBV	1497664	2134348	32.54%	5.180%
17	17.539	2437	2440	2449	rVV	554308	830897	12.67%	2.016%
18	17.633	2452	2456	2460	rVB	108156	153417	2.34%	0.372%
19	17.898	2497	2501	2505	rVB	55132	67349	1.03%	0.163%
20	17.969	2510	2513	2517	rVV	64138	69281	1.06%	0.168%
21	18.351	2574	2578	2583	rBV2	172525	261087	3.98%	0.634%
22	18.398	2583	2586	2593	rVB2	110048	153337	2.34%	0.372%
23	18.545	2606	2611	2614	rBV2	86738	152762	2.33%	0.371%
24	18.633	2623	2626	2630	rBV2	78057	98967	1.51%	0.240%
25	19.239	2725	2729	2732	rBV2	128719	163292	2.49%	0.396%
26	19.492	2767	2772	2777	rBV	1041678	1277792	19.48%	3.101%
27	19.810	2821	2826	2828	rBV3	165454	324611	4.95%	0.788%
28	19.845	2828	2832	2840	rVB	914116	1226945	18.70%	2.977%
29	20.033	2858	2864	2869	rBV	5222054	6559591	100.00%	15.918%
30	20.310	2909	2911	2917	rVB2	217756	296098	4.51%	0.719%
31	20.792	2991	2993	2997	rVB	162597	164984	2.52%	0.400%
32	21.251	3067	3071	3075	rBV2	596119	745006	11.36%	1.808%
33	21.574	3120	3126	3131	rBV2	1925090	3254636	49.62%	7.898%
34	21.692	3142	3146	3152	rBV	1448665	2304708	35.13%	5.593%
35	24.133	3556	3561	3569	rVB2	1131094	2347915	35.79%	5.698%

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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

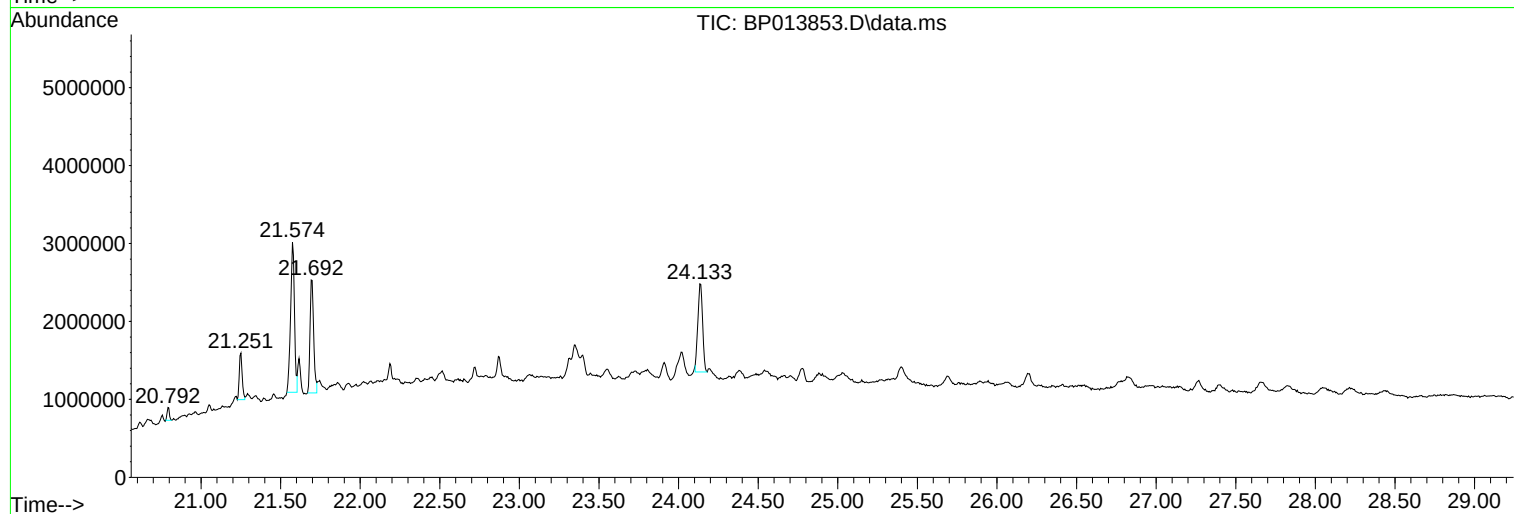
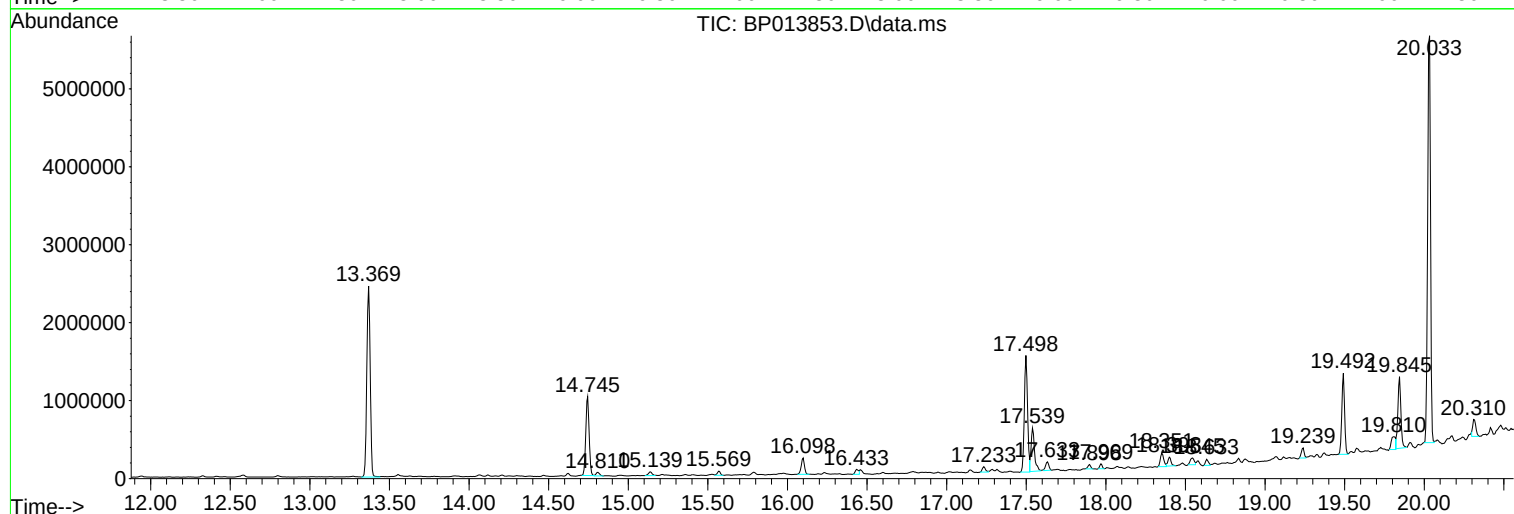
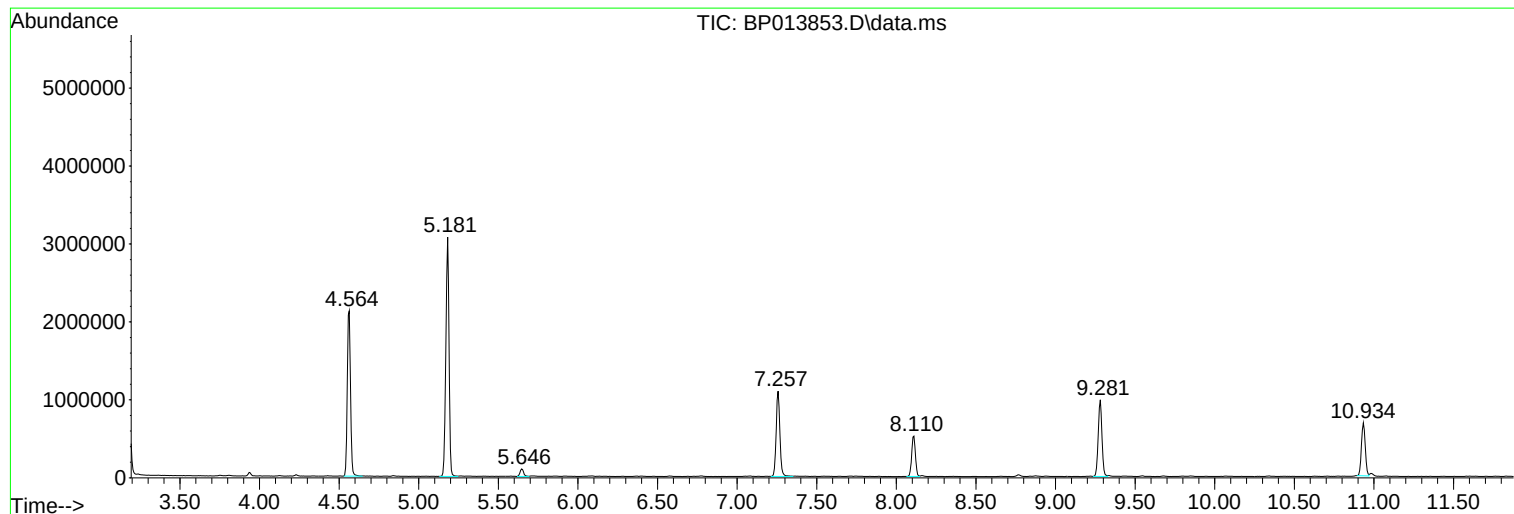
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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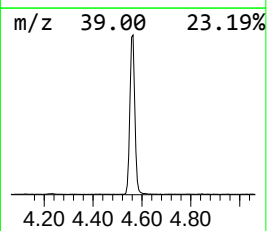
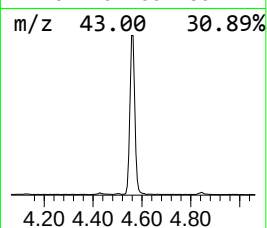
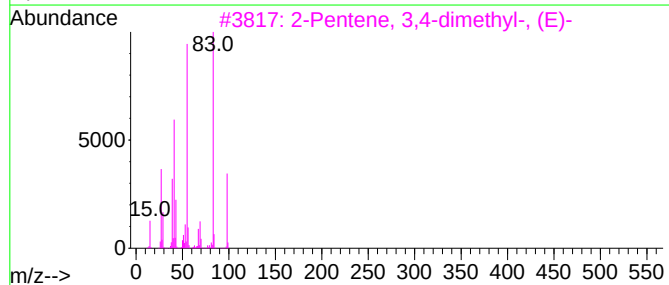
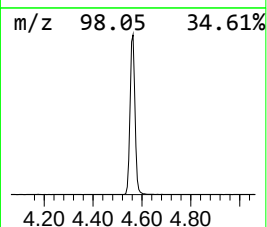
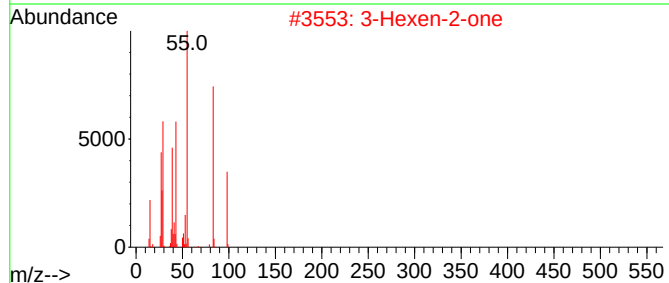
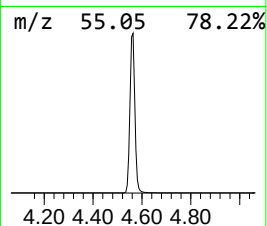
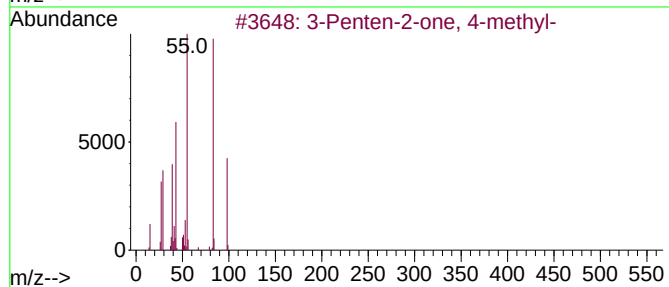
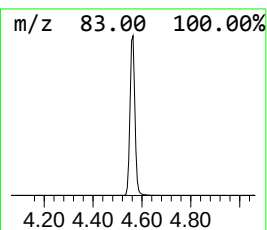
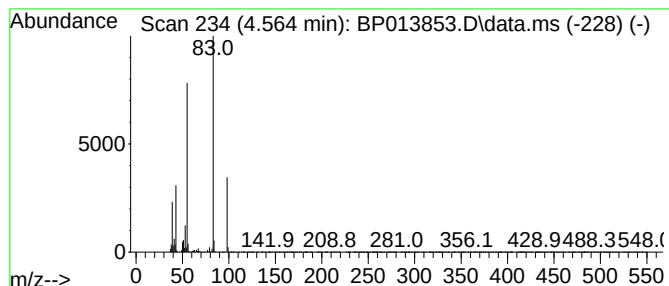
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.564	70.69 ng	2961750	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	91
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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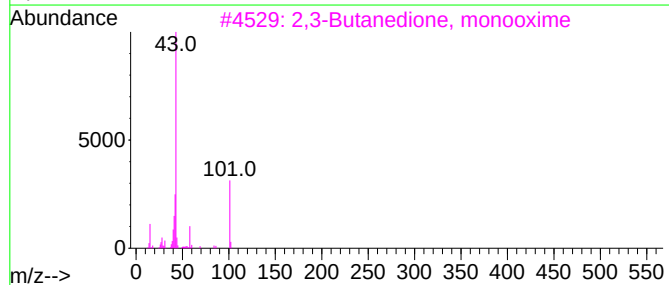
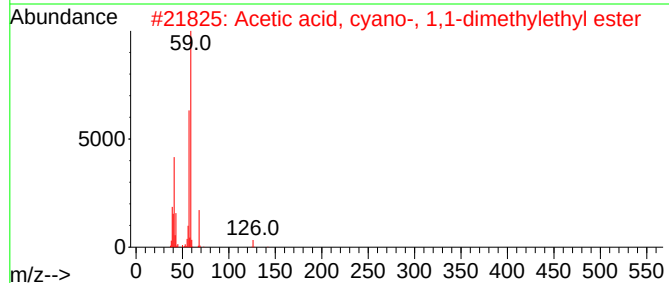
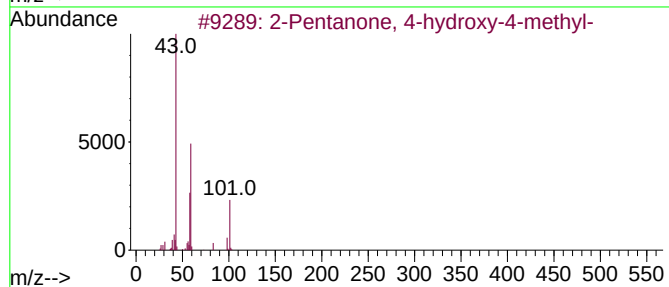
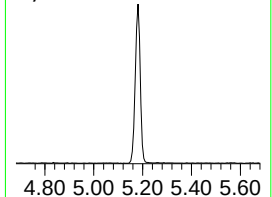
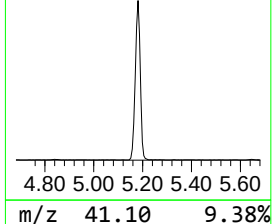
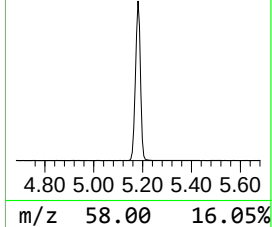
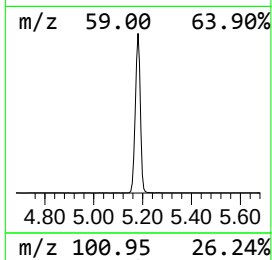
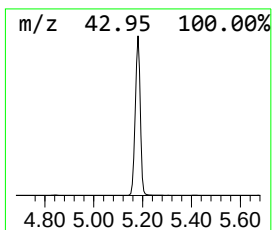
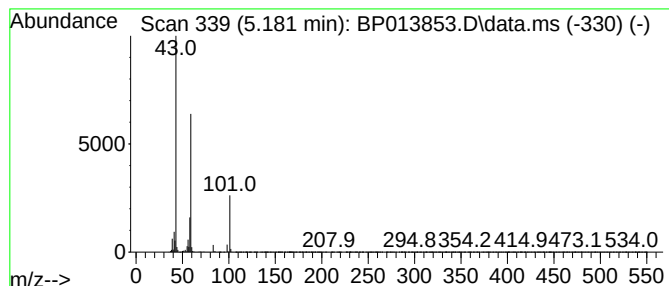
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	103.60 ng	4340520	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			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
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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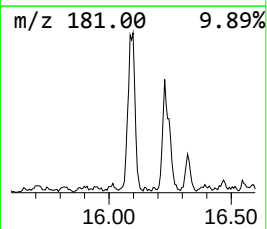
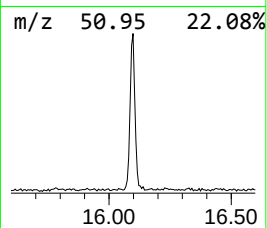
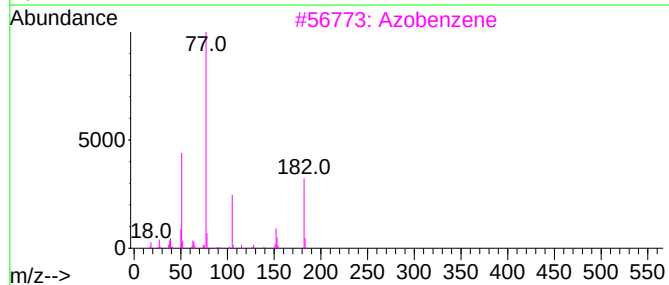
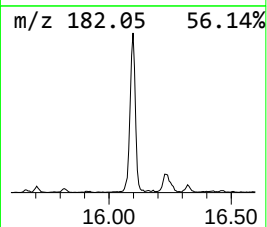
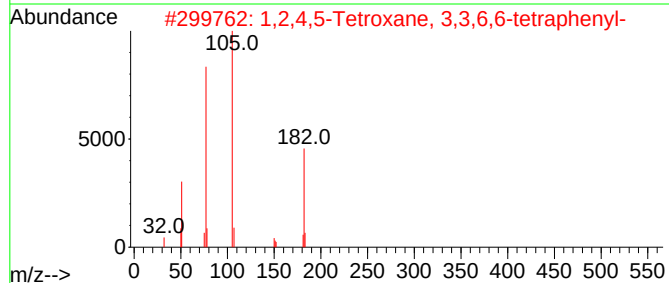
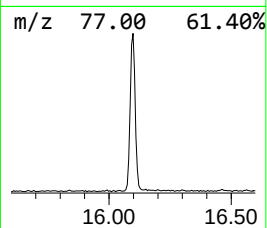
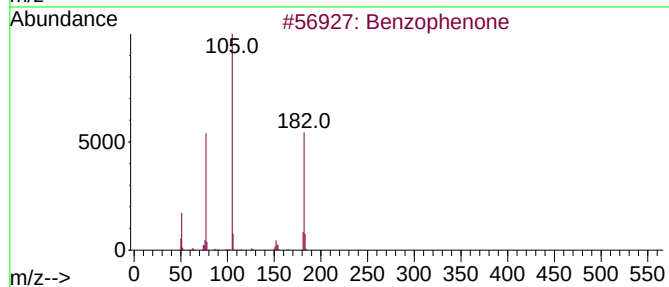
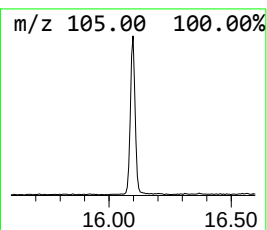
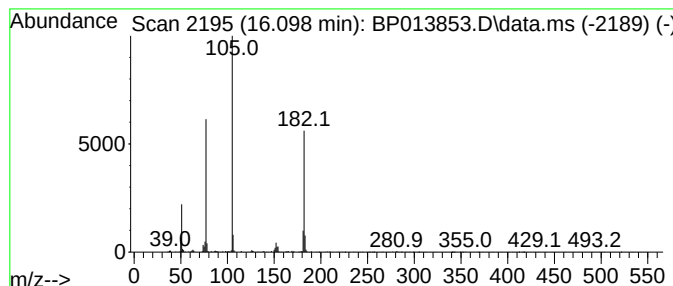
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	3.96 ng	295388	Acenaphthene-d10	14.745

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			Azobenzene	182	C12H10N2	000103-33-3	59
4			Isovanillic acid, 0-methoxycarbo...	226	C10H10O6	1000487-72-5	43
5			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	42



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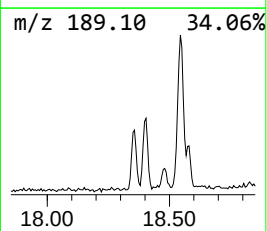
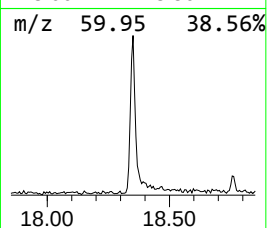
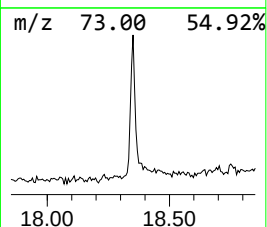
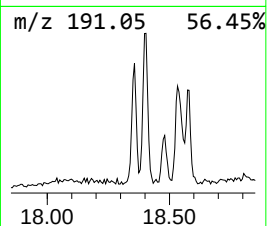
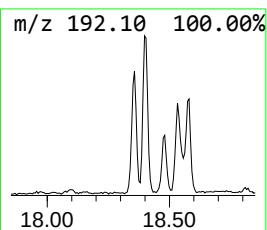
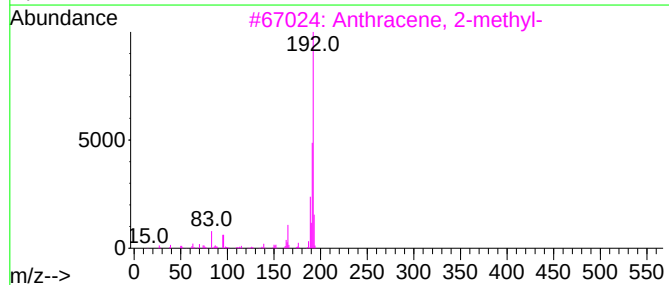
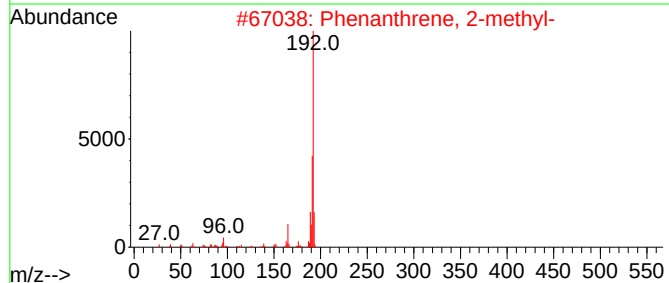
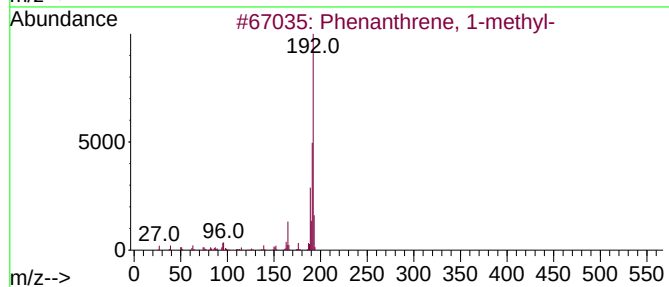
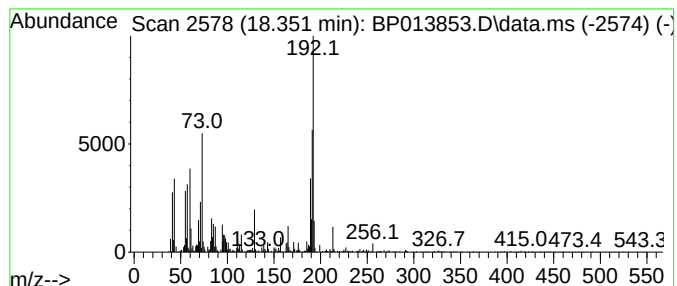
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	2.45 ng	261087	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4			Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	89



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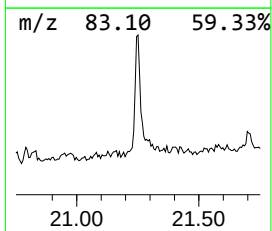
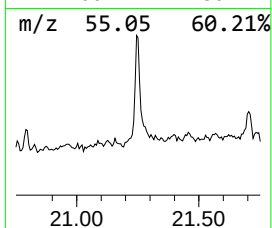
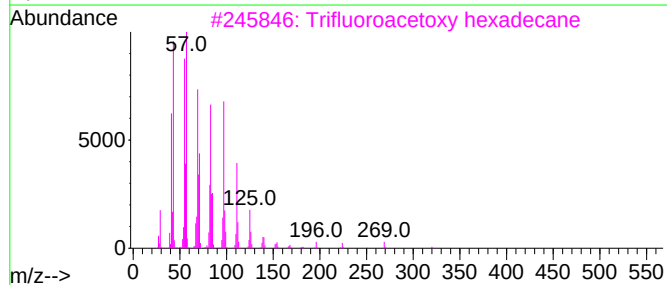
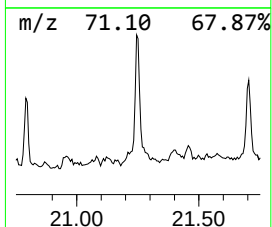
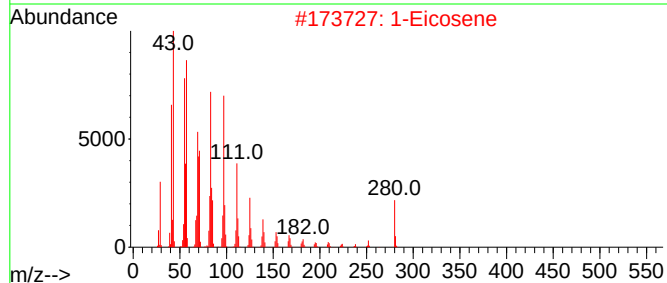
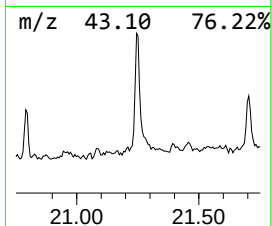
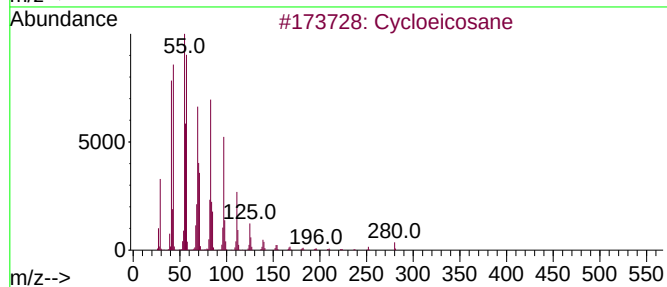
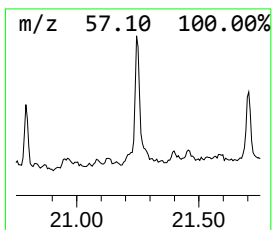
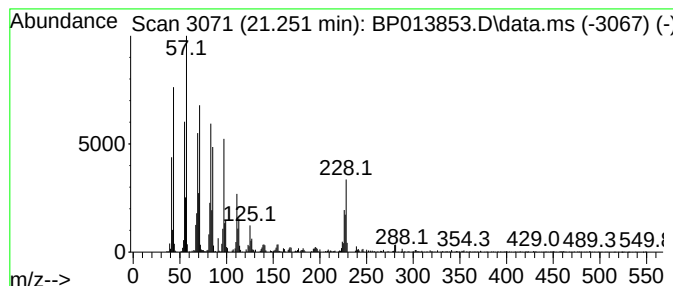
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	4.58 ng	745006	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	89
2			1-Eicosene	280	C20H40	003452-07-1	89
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
4			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	83
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013853.D
Acq On : 17 Feb 2023 19:41
Operator : CG/JU
Sample : 01586-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-4

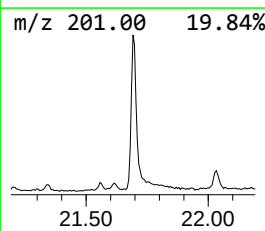
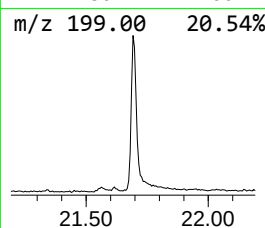
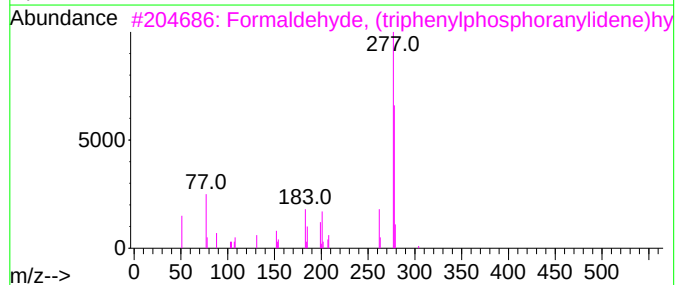
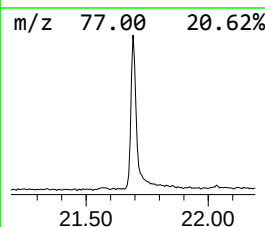
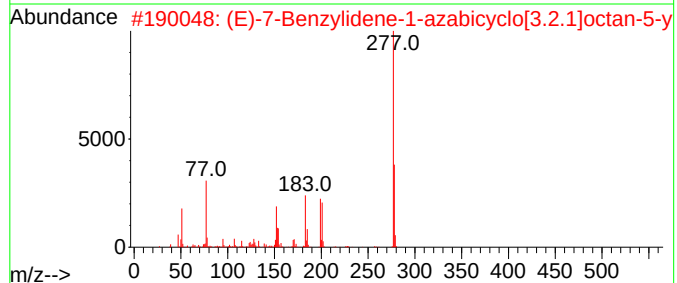
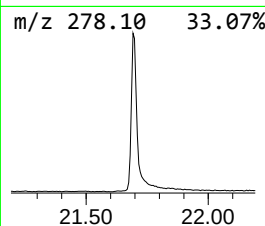
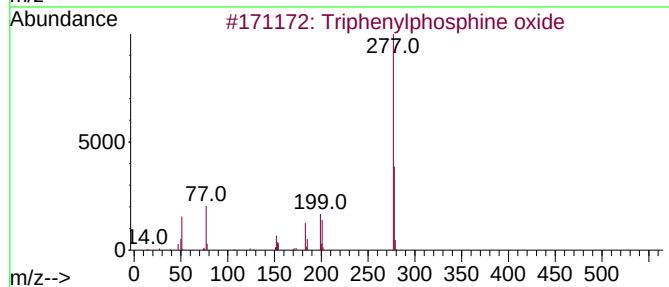
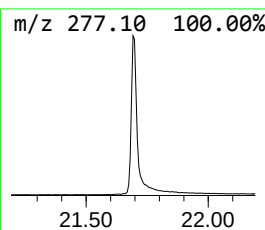
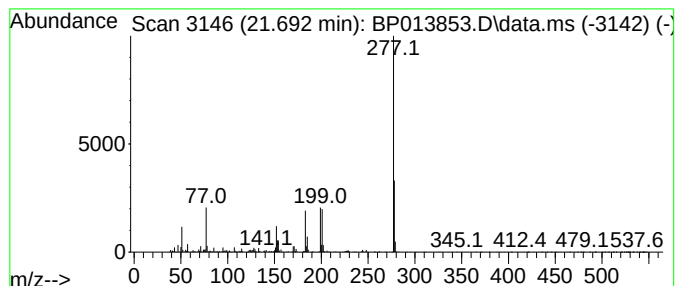
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.692	14.16 ng	2304710	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2			(E)-7-Benzylidene-1-azabicyclo[3.1.0]hex-5-en-2-ylidene triphenylphosphorane	293	C15H19NO3S	1000483-83-4	83
3			Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	42
4			Vanadium, cycloheptatrienyl-(pentamethyl)-	277	C17H22V	1000155-20-5	25
5			1H-Indole-3-acetic acid, 5-[(trimethylsilyl)ethynyl]-	277	C14H19NO3Si	072101-35-0	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013853.D
Acq On : 17 Feb 2023 19:41
Operator : CG/JU
Sample : 01586-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.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
3-Penten-2-one,...	4.564	70.7	ng	2961750	1	8.110	837979	20.0
2-Pentanone, 4-...	5.181	103.6	ng	4340520	1	8.110	837979	20.0
Benzophenone	16.098	4.0	ng	295388	3	14.745	1492520	20.0
Phenanthrene, 1...	18.351	2.5	ng	261087	4	17.498	2134350	20.0
Cycloeicosane	21.251	4.6	ng	745006	5	21.574	3254640	20.0
Triphenylphosph...	21.692	14.2	ng	2304710	5	21.574	3254640	20.0