

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
 Data File : BP013854.D
 Acq On : 17 Feb 2023 20:15
 Operator : CG/JU
 Sample : 01586-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-1

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: BP013854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.934	123	127	133	rVB	66976	89730	1.70%	0.233%
2	4.564	228	234	248	rBV	3657109	4971015	94.37%	12.884%
3	5.181	331	339	350	rBV	3581576	5267774	100.00%	13.654%
4	5.646	411	418	424	rBV	54791	85096	1.62%	0.221%
5	7.258	685	692	708	rVB	679741	1097604	20.84%	2.845%
6	8.111	827	837	844	rBV	533379	867109	16.46%	2.247%
7	9.281	1028	1036	1043	rBV	712608	1157397	21.97%	3.000%
8	10.934	1300	1317	1323	rBV	671669	1148278	21.80%	2.976%
9	10.987	1323	1326	1333	rVB	45787	71783	1.36%	0.186%
10	12.581	1588	1597	1602	rVB	31489	56774	1.08%	0.147%
11	13.369	1722	1731	1738	rBV	2044831	2958678	56.17%	7.669%
12	14.746	1953	1965	1971	rBV	1126644	1693427	32.15%	4.389%
13	14.810	1971	1976	1983	rVB	55508	90182	1.71%	0.234%
14	15.140	2027	2032	2038	rVB2	41813	65048	1.23%	0.169%
15	15.569	2101	2105	2110	rVB2	44791	61013	1.16%	0.158%
16	16.098	2189	2195	2203	rVB	168458	247076	4.69%	0.640%
17	16.440	2248	2253	2254	rBV	50878	68309	1.30%	0.177%
18	17.234	2384	2388	2393	rBV3	62629	90160	1.71%	0.234%
19	17.498	2427	2433	2437	rBV	1481448	2124504	40.33%	5.506%
20	17.540	2437	2440	2448	rVV	351926	551273	10.47%	1.429%
21	17.634	2452	2456	2460	rVB	70366	101851	1.93%	0.264%
22	17.969	2510	2513	2516	rVB	52616	57150	1.08%	0.148%
23	18.351	2574	2578	2583	rBV2	141441	210024	3.99%	0.544%
24	18.404	2584	2587	2590	rVB	65790	84631	1.61%	0.219%
25	18.545	2607	2611	2614	rBV2	60691	98511	1.87%	0.255%
26	18.634	2623	2626	2631	rBV	58652	79214	1.50%	0.205%
27	19.239	2726	2729	2733	rVB	102824	120032	2.28%	0.311%
28	19.492	2768	2772	2778	rVB	683622	842430	15.99%	2.183%
29	19.798	2821	2824	2828	rBV2	124428	227801	4.32%	0.590%
30	19.845	2828	2832	2839	rVB	639405	860299	16.33%	2.230%
31	20.034	2859	2864	2869	rBV	3865549	4895538	92.93%	12.689%
32	20.316	2909	2912	2917	rVB2	201133	263284	5.00%	0.682%
33	21.251	3067	3071	3076	rBV2	543844	687566	13.05%	1.782%
34	21.580	3121	3127	3131	rBV2	1736097	2776799	52.71%	7.197%
35	21.698	3142	3147	3153	rBV	1368943	2178306	41.35%	5.646%
36	24.139	3557	3562	3569	rVB2	1187114	2336169	44.35%	6.055%

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

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

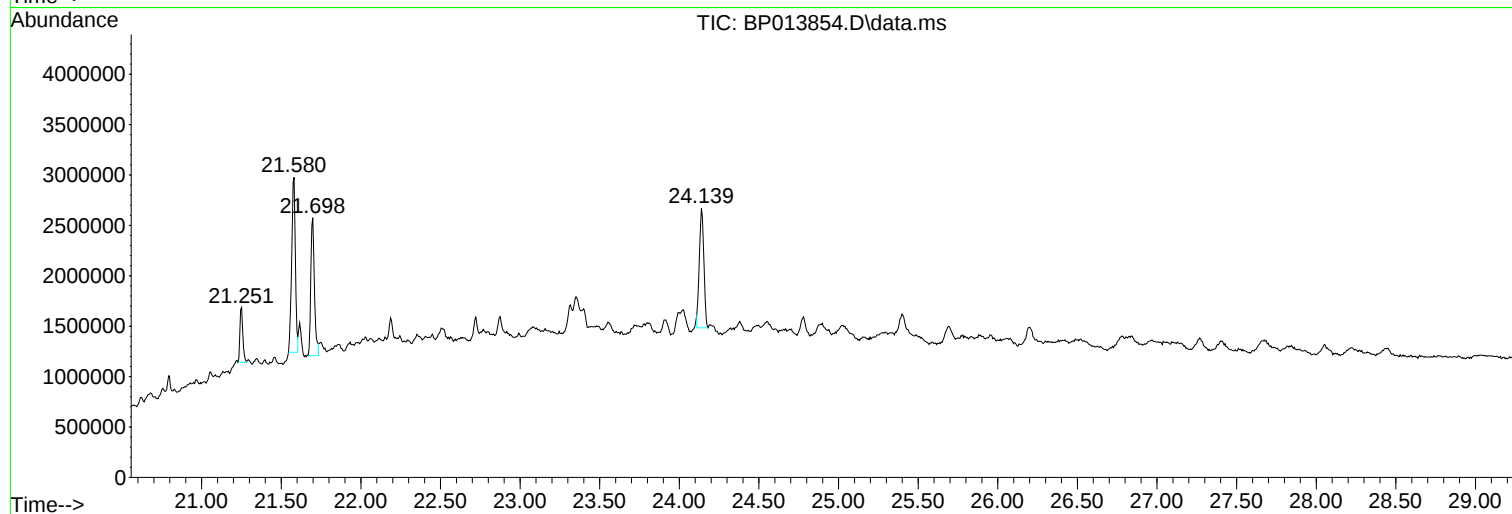
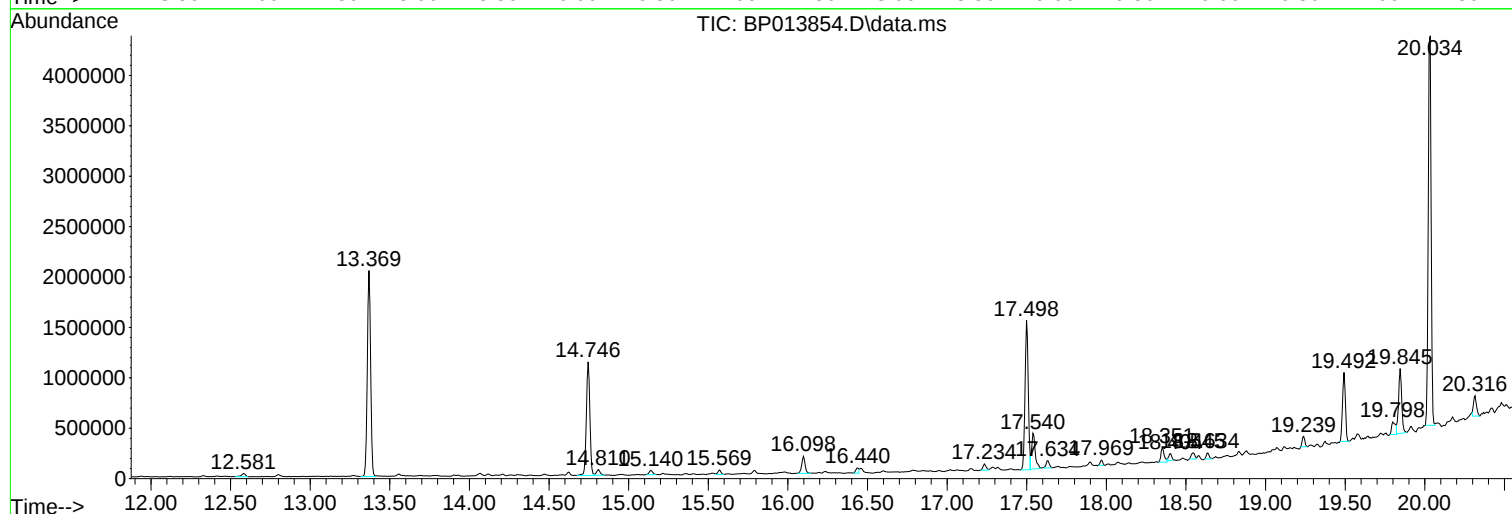
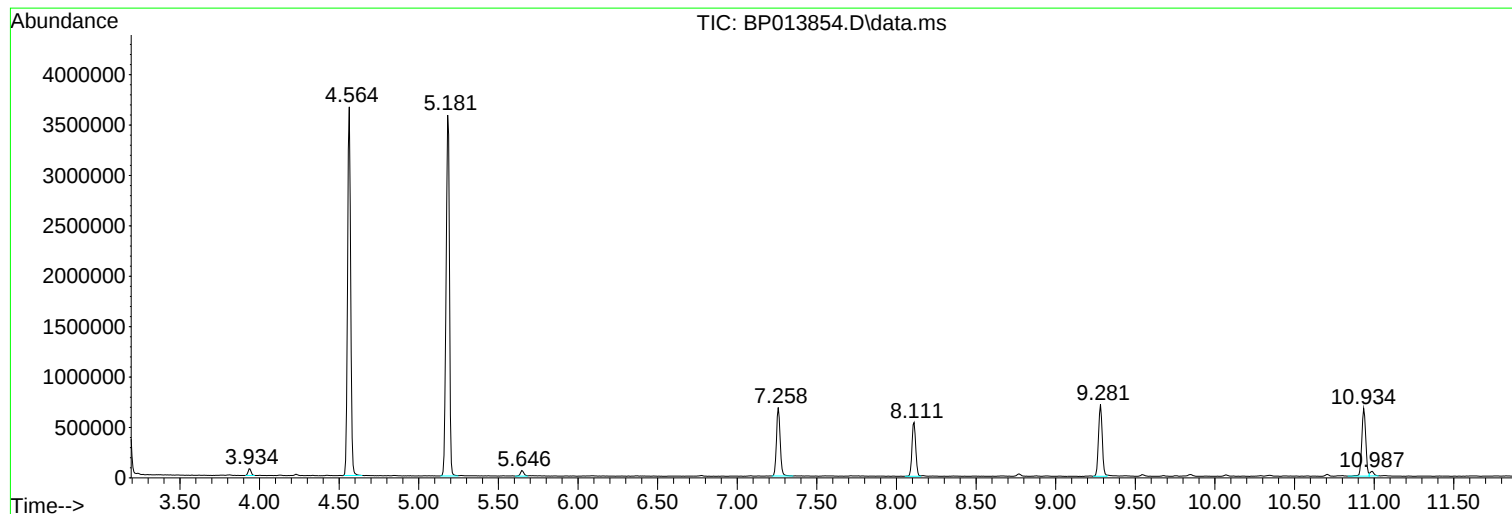
Sum of corrected areas: 38581835

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

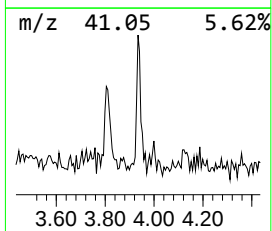
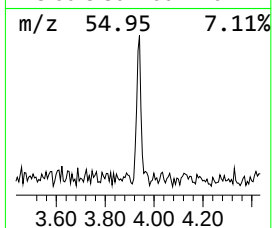
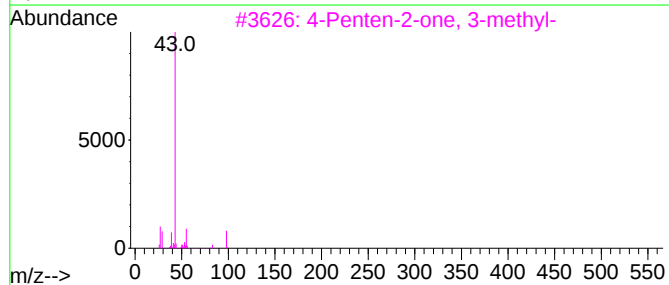
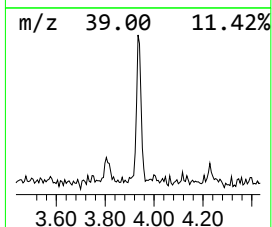
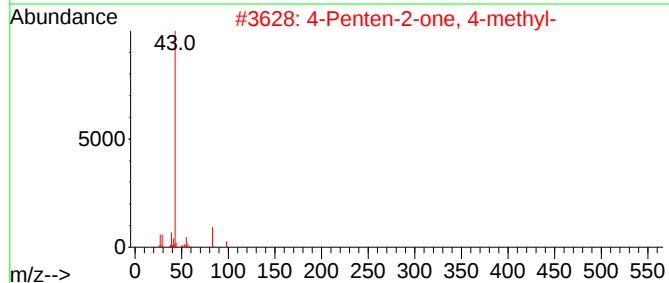
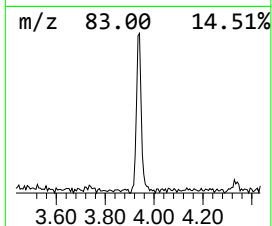
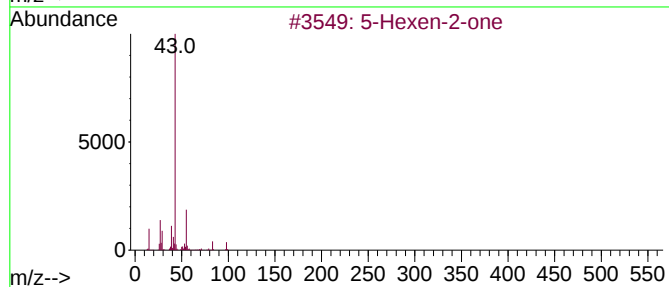
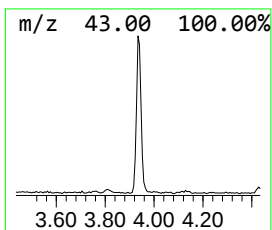
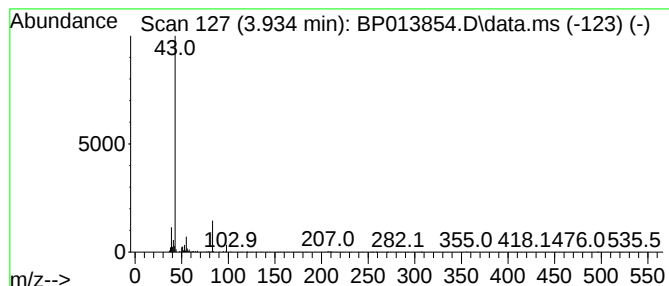
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.934 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.934	2.07 ng	89730	1,4-Dichlorobenzene-d4	8.111

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Hexen-2-one	98	C6H10O	000109-49-9	43
2			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	43
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	25
4			2-Vinylethyl acetate	114	C6H10O2	001576-84-7	23
5			2,4-Pentanedione, 3-methyl-	114	C6H10O2	000815-57-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

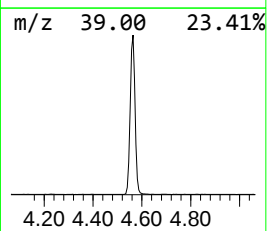
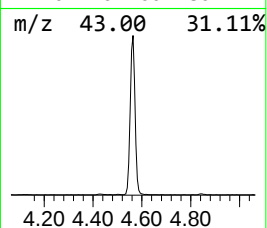
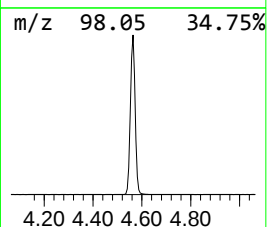
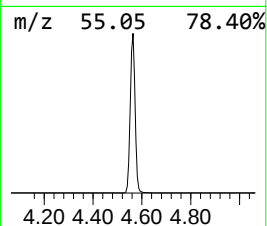
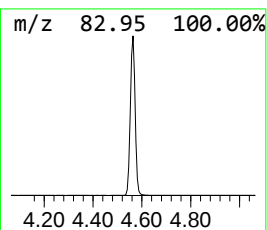
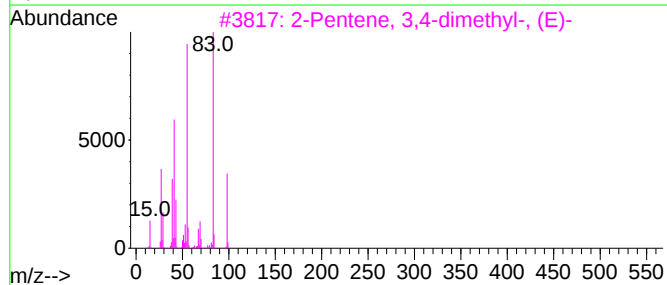
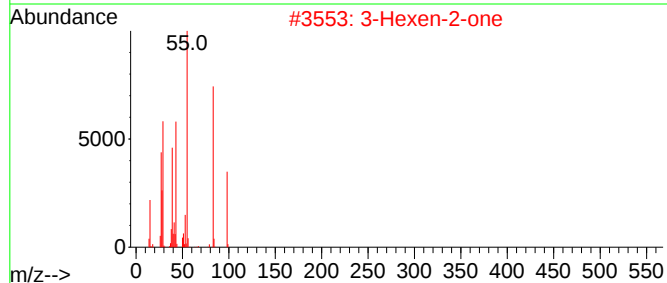
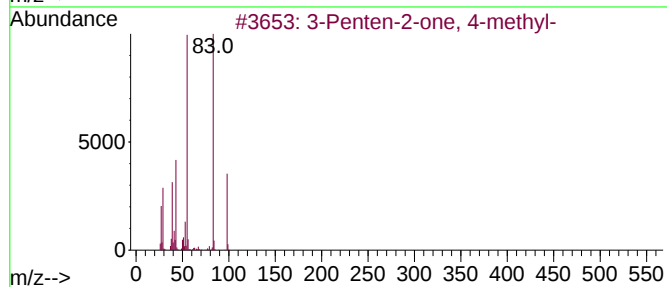
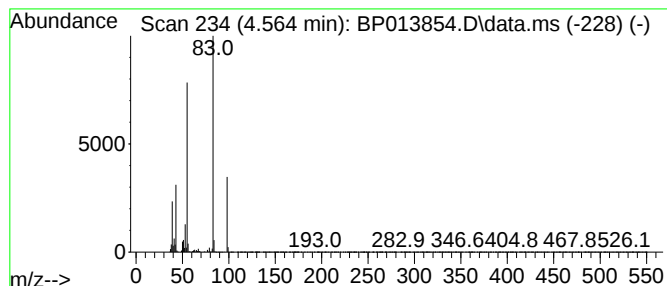
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.564	114.66 ng	4971020	1,4-Dichlorobenzene-d4	8.111

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

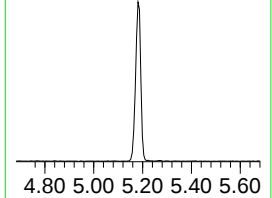
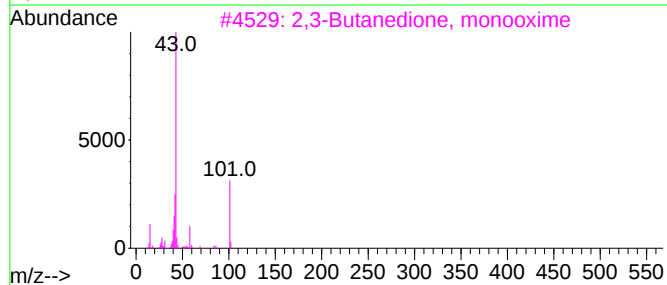
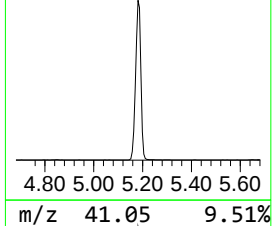
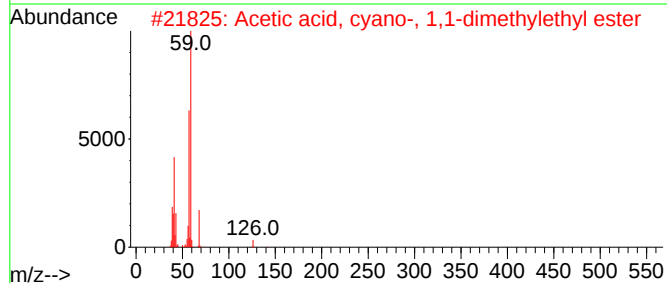
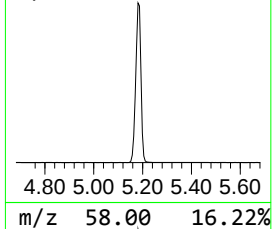
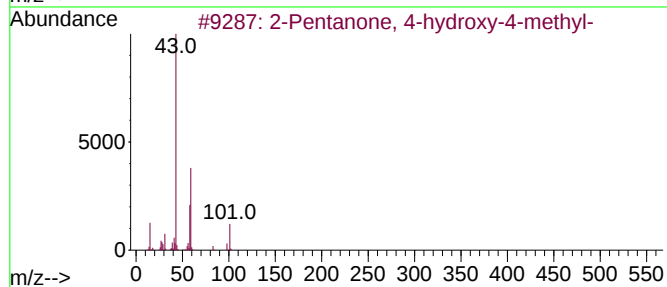
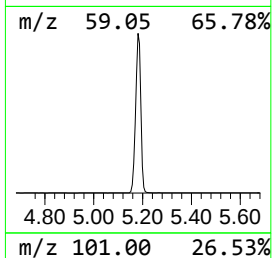
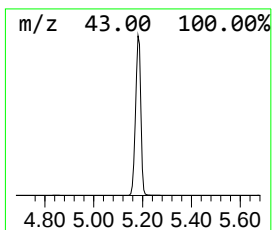
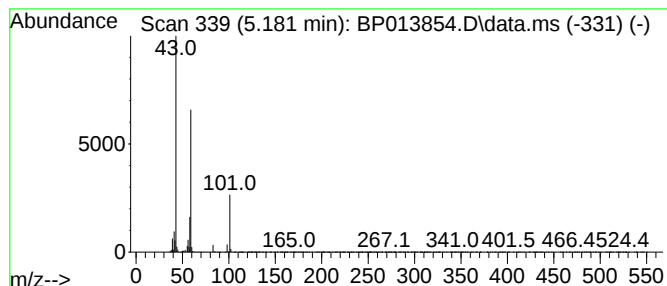
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	121.50 ng	5267770	1,4-Dichlorobenzene-d4	8.111

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	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			Acetone	58	C3H6O	000067-64-1	10
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

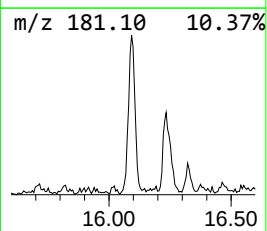
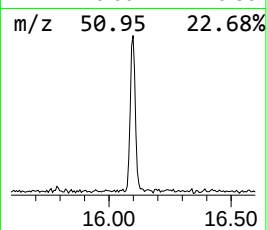
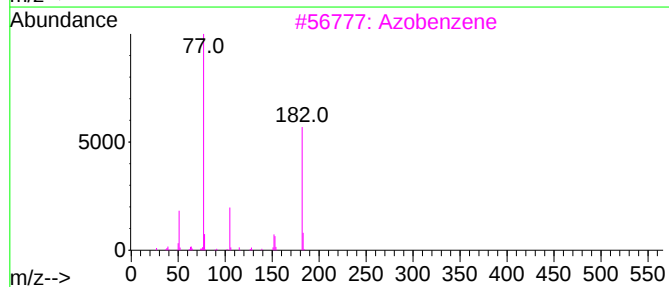
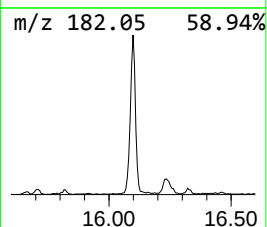
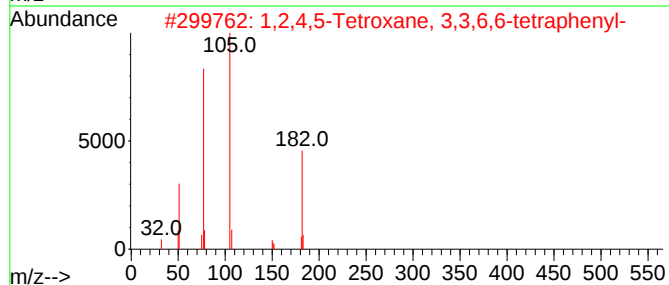
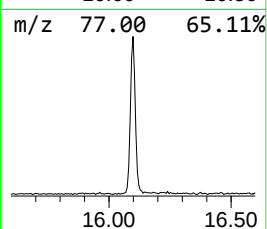
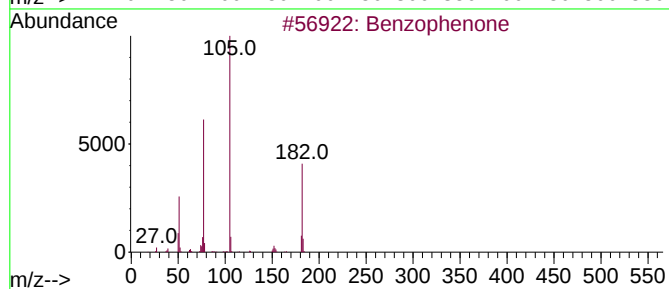
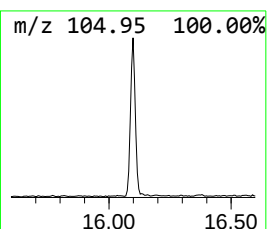
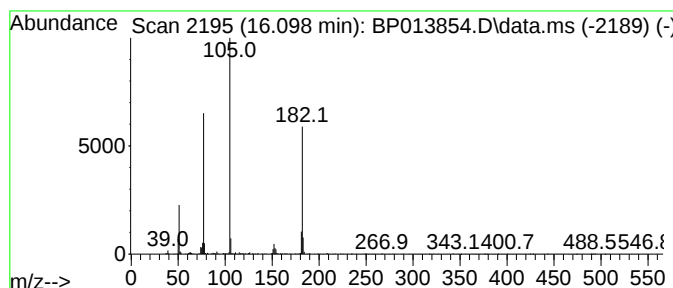
Instrument :
BNA_P
ClientSampleId :
COMP-1

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 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.098	2.92 ng	247076	Acenaphthene-d10	14.746	
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	64
3	Azobenzene	182	C12H10N2	000103-33-3	59
4	1,2,4-Triazolo[4,3-b]pyridazine,...	182	C7H7ClN4	028593-26-2	38
5	[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

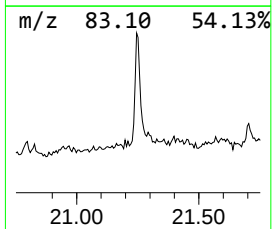
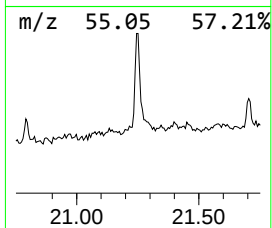
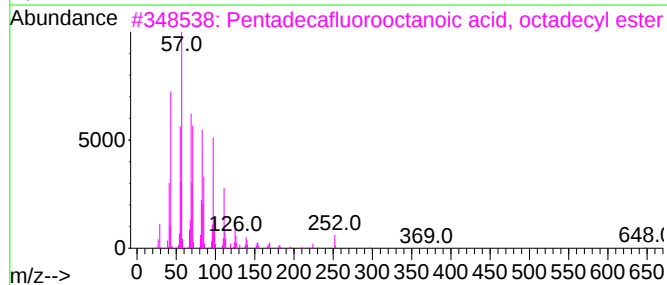
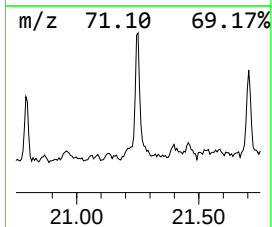
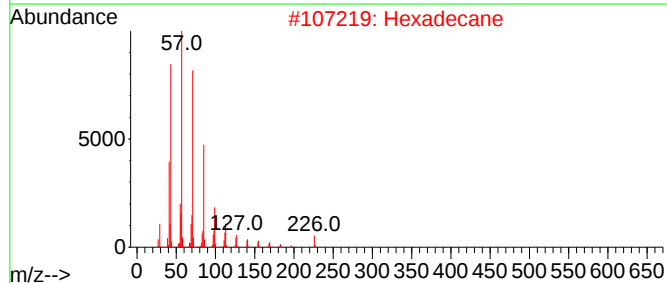
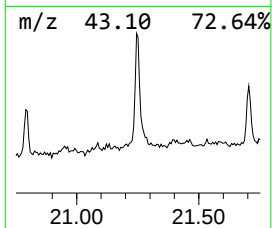
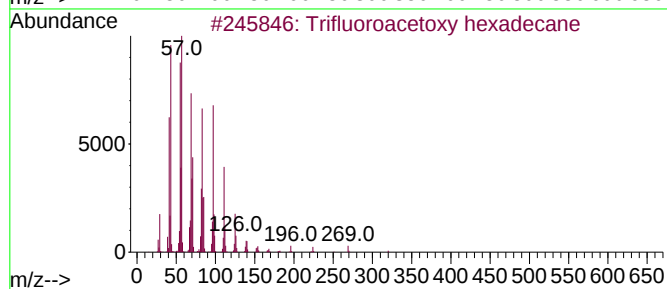
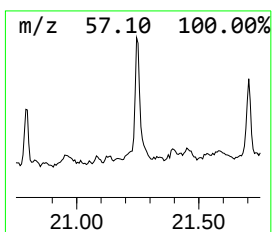
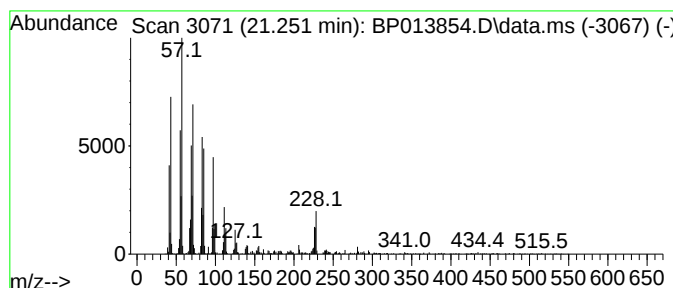
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	4.95 ng	687566	Chrysene-d12	21.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
2			Hexadecane	226	C16H34	000544-76-3	81
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	78
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	70
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
Data File : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

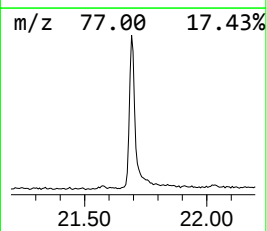
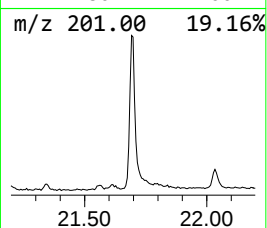
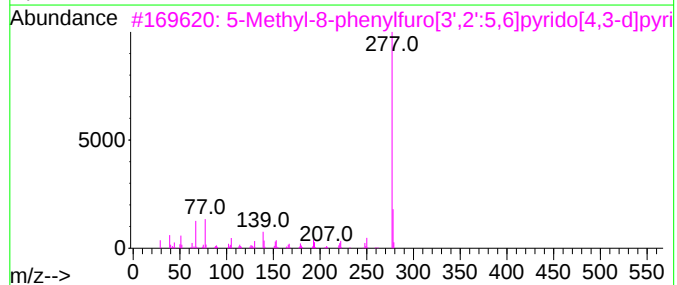
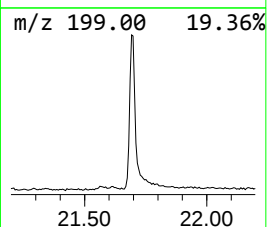
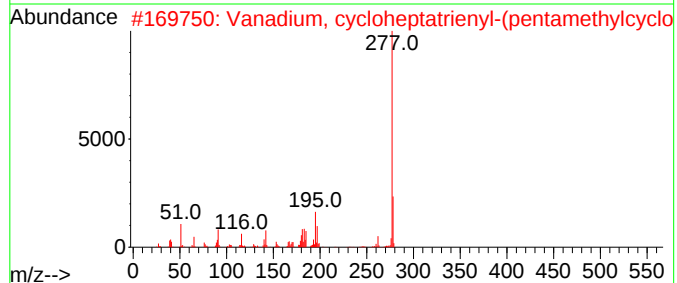
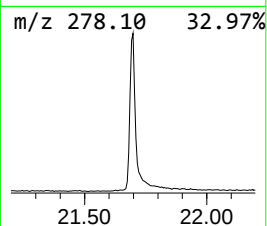
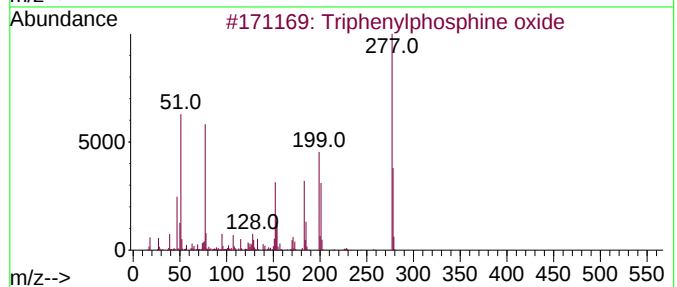
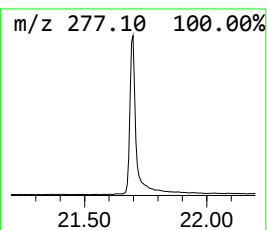
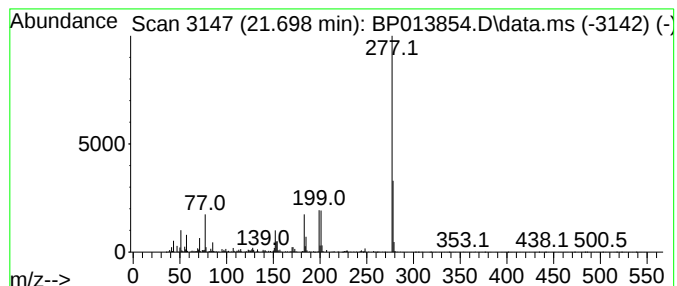
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
21.698	15.69 ng	2178310	Chrysene-d12	21.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	40
3			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	23
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 : BP013854.D
Acq On : 17 Feb 2023 20:15
Operator : CG/JU
Sample : 01586-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-1

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
unknown3.934	3.934	2.1	ng	89730	1	8.111	867109	20.0
3-Penten-2-one,...	4.564	114.7	ng	4971020	1	8.111	867109	20.0
2-Pentanone, 4-...	5.181	121.5	ng	5267770	1	8.111	867109	20.0
Benzophenone	16.098	2.9	ng	247076	3	14.746	1693430	20.0
Trifluoroacetox...	21.251	5.0	ng	687566	5	21.581	2776800	20.0
Triphenylphosph...	21.698	15.7	ng	2178310	5	21.581	2776800	20.0