

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
 Data File : BF125637.D
 Acq On : 24 Sep 2021 23:56
 Operator : JU/CG
 Sample : M3916-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CONC-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_F\METHODS\8270-BF092421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125637.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	30	rVB	1367332	1755765	35.34%	5.197%
2	4.504	401	411	418	rBV	611165	663399	13.35%	1.964%
3	5.116	505	515	522	rBV	218808	269626	5.43%	0.798%
4	5.504	576	581	585	rBV	3451158	3612421	72.71%	10.692%
5	6.504	746	751	754	rBV	3538088	3757328	75.62%	11.121%
6	6.886	812	816	819	rBV	1598487	1248079	25.12%	3.694%
7	7.445	905	911	914	rBV	2654526	2450225	49.32%	7.252%
8	8.063	1013	1016	1024	rBV	129422	108431	2.18%	0.321%
9	8.169	1029	1034	1037	rBV	1909685	1749590	35.21%	5.178%
10	9.245	1211	1217	1220	rBV	5383402	4968412	100.00%	14.705%
11	9.922	1328	1332	1335	rBV	2562430	1948007	39.21%	5.766%
12	10.704	1461	1465	1469	rBV	2539853	2266024	45.61%	6.707%
13	11.180	1543	1546	1550	rVB	128997	99742	2.01%	0.295%
14	11.404	1580	1584	1587	rBV	2169510	1762264	35.47%	5.216%
15	12.992	1849	1854	1857	rBV	3985524	3640992	73.28%	10.777%
16	13.851	1996	2000	2002	rBV	180911	143187	2.88%	0.424%
17	13.886	2002	2006	2009	rBV2	62022	87245	1.76%	0.258%
18	14.039	2027	2032	2036	rBV	1324761	1130181	22.75%	3.345%
19	14.180	2052	2056	2059	rBV	153978	137610	2.77%	0.407%
20	14.215	2059	2062	2065	rVV	246965	222475	4.48%	0.658%
21	14.245	2065	2067	2069	rVV	85542	67681	1.36%	0.200%
22	14.268	2069	2071	2075	rVB	94555	75347	1.52%	0.223%
23	15.515	2278	2283	2287	rBV	1029893	1221981	24.60%	3.617%
24	16.245	2403	2407	2414	rVB4	72874	132409	2.67%	0.392%
25	16.686	2478	2482	2488	rVB3	105513	187573	3.78%	0.555%
26	17.280	2579	2583	2590	rVB7	44560	80301	1.62%	0.238%

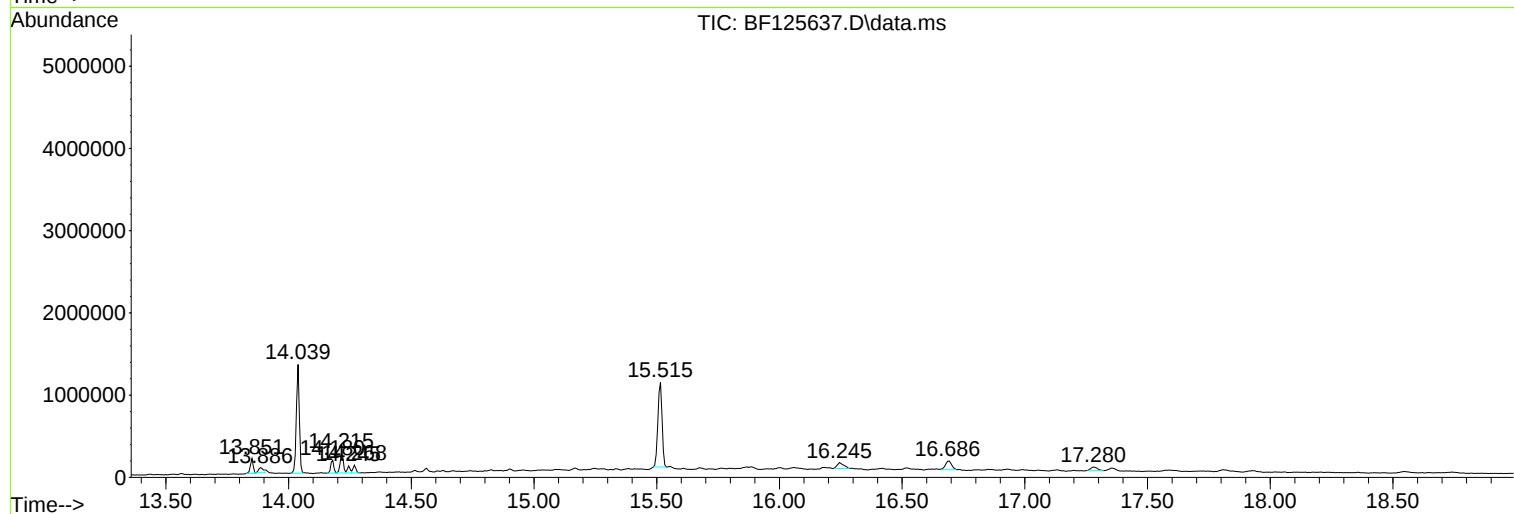
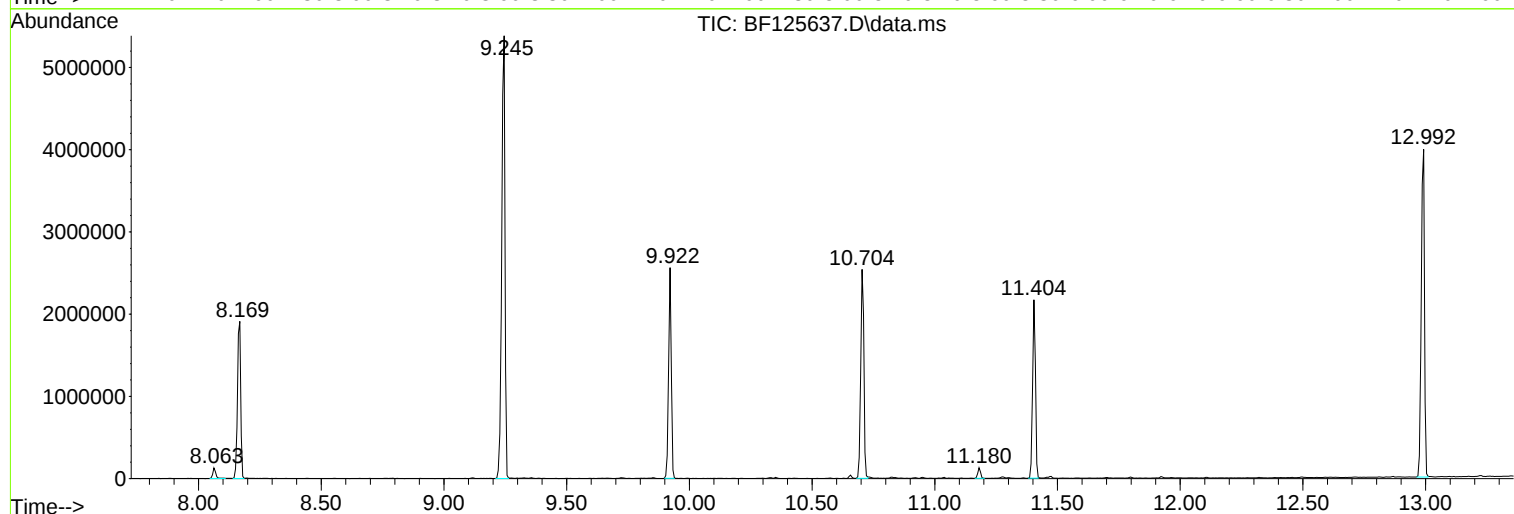
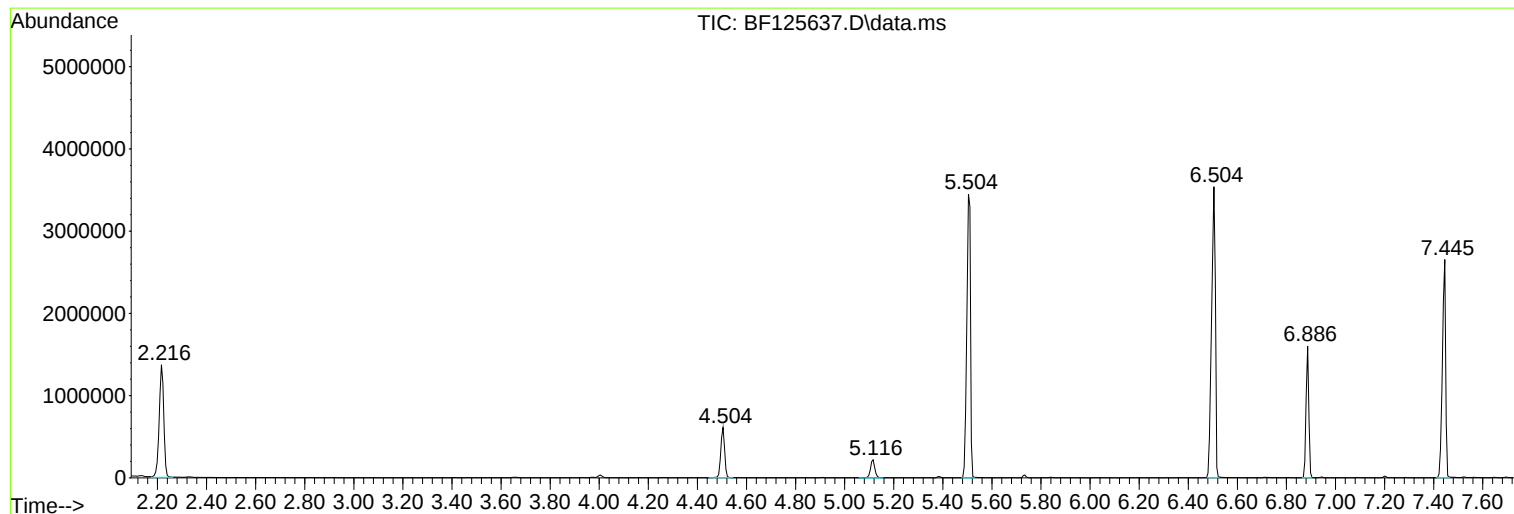
Sum of corrected areas: 33786295

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

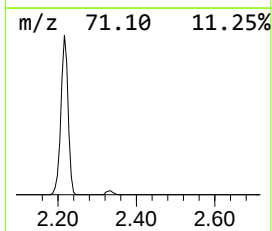
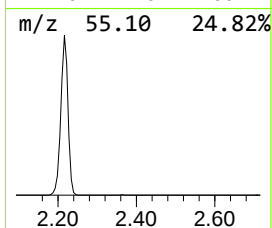
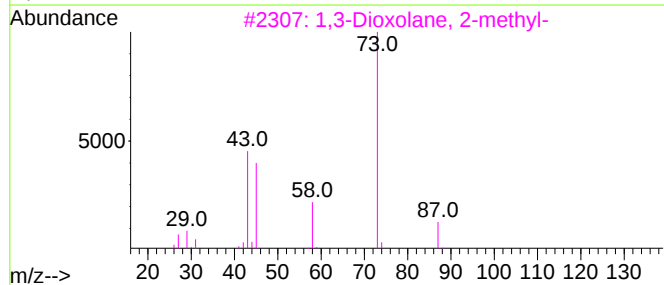
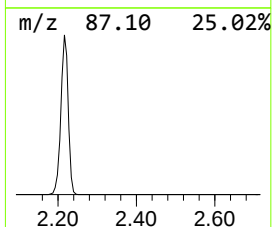
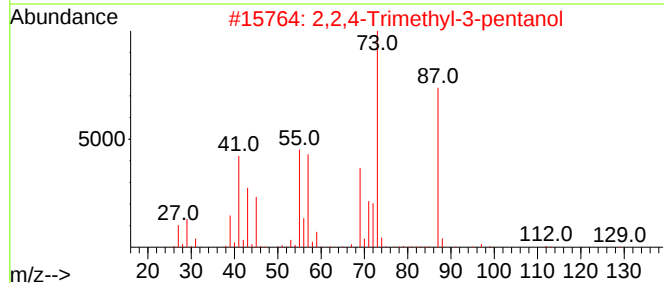
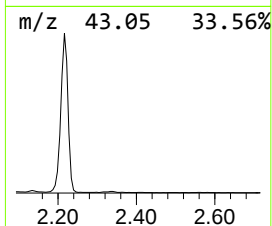
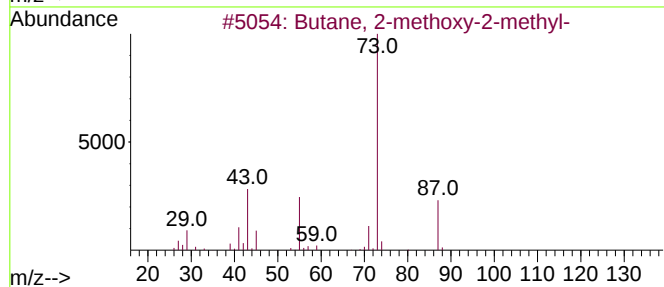
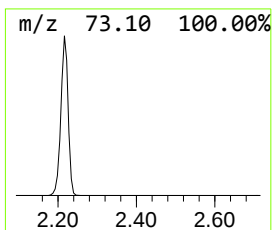
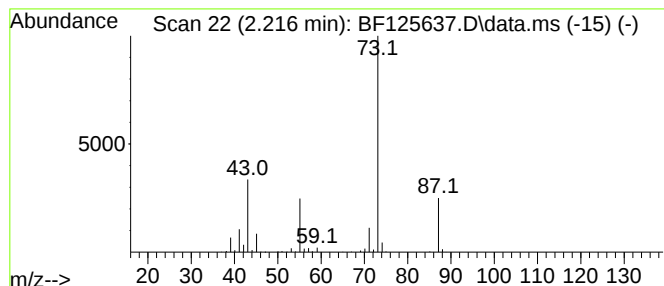
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	28.14 ng	1755770	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

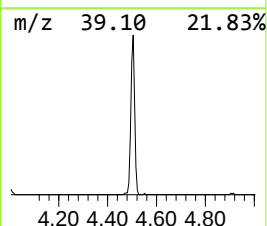
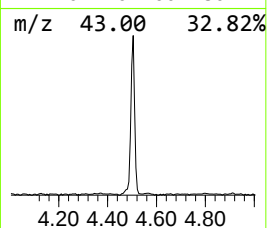
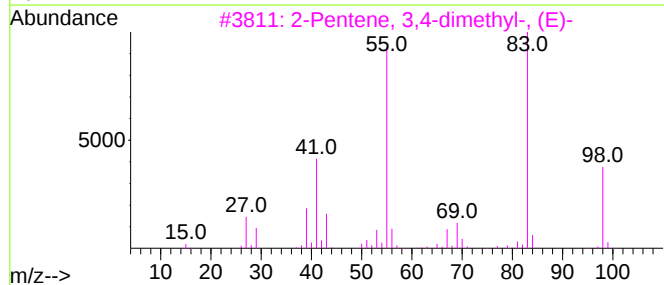
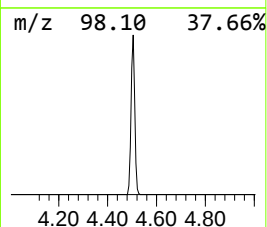
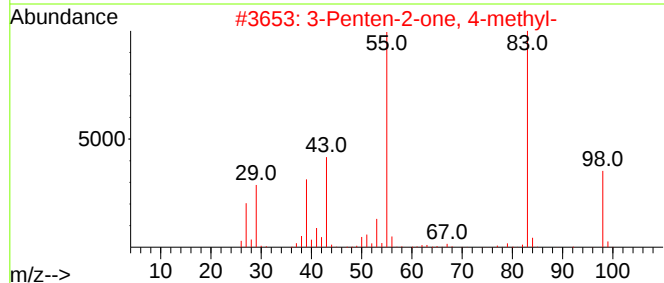
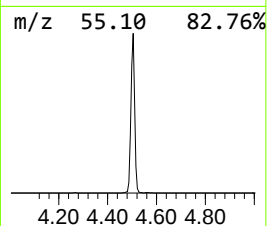
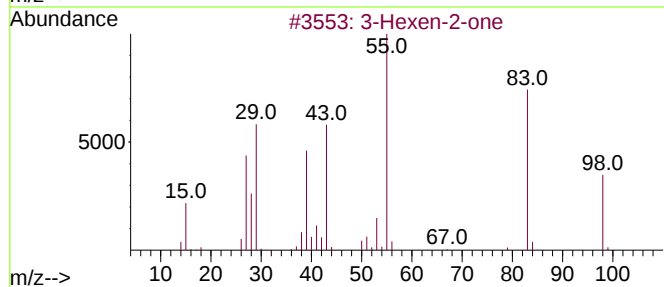
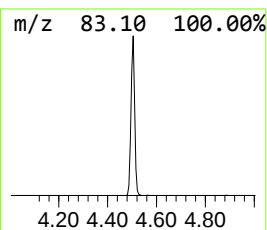
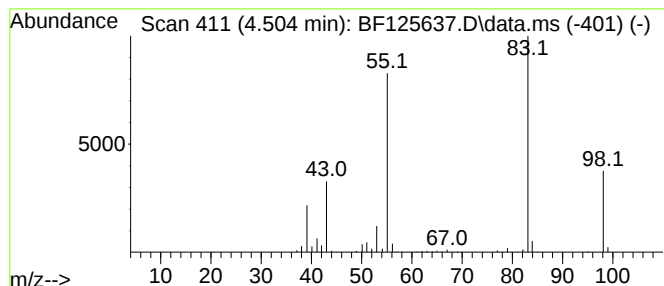
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	10.63 ng	663399	1,4-Dichlorobenzene-d4	6.886

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

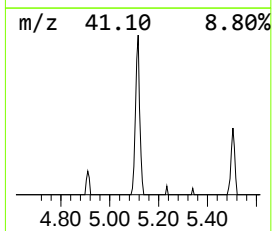
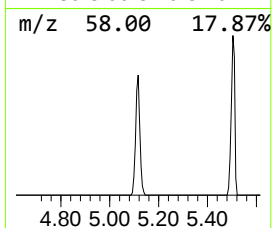
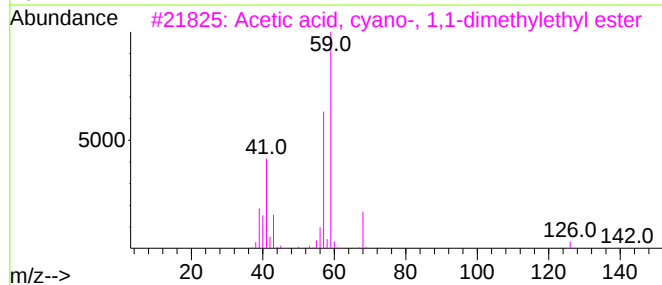
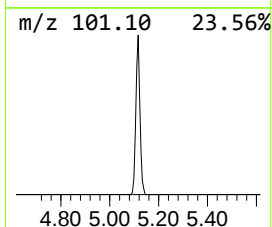
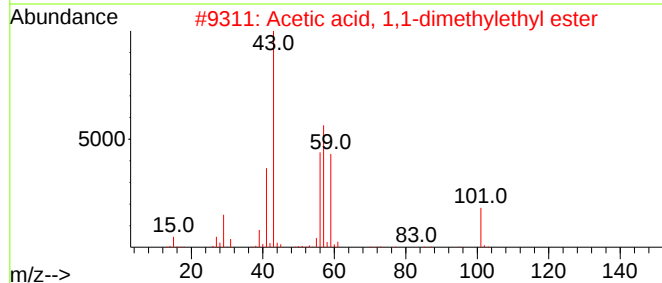
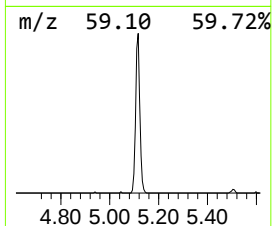
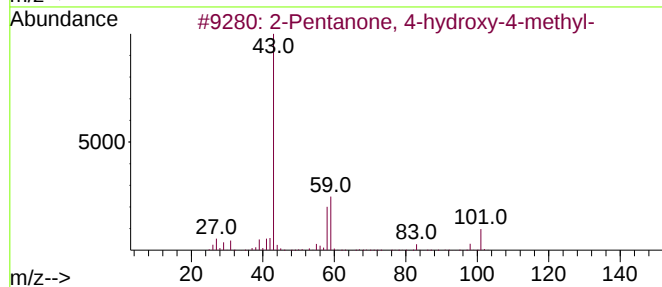
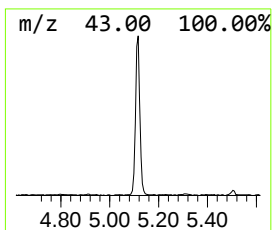
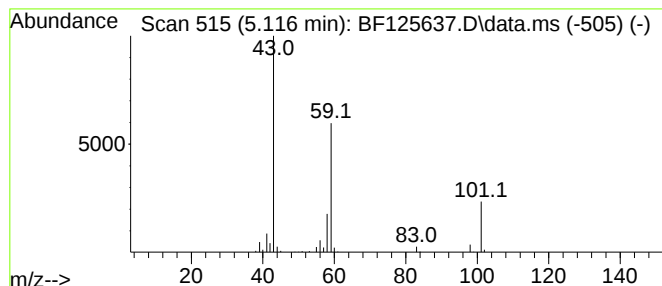
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	4.32 ng	269626	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
CONC-2

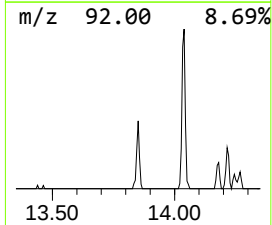
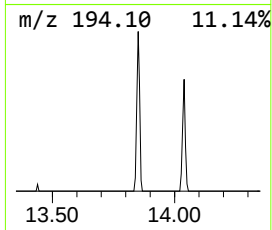
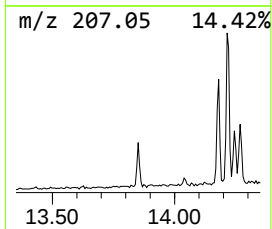
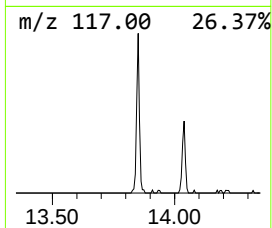
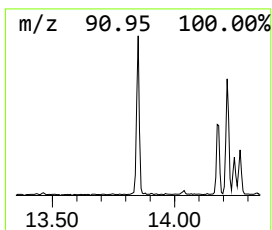
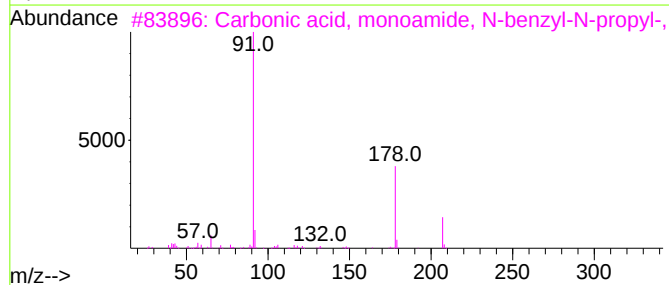
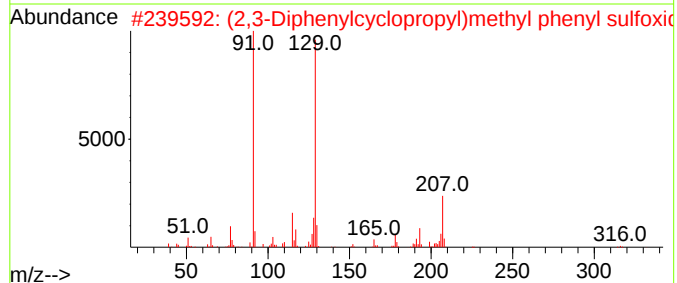
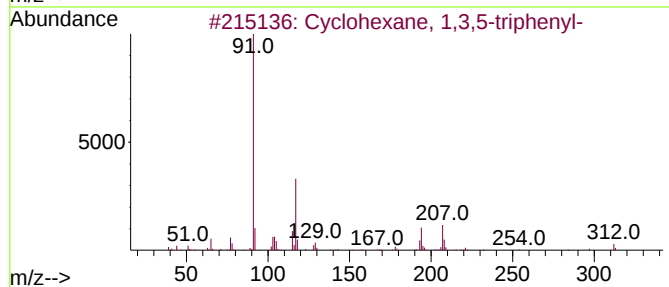
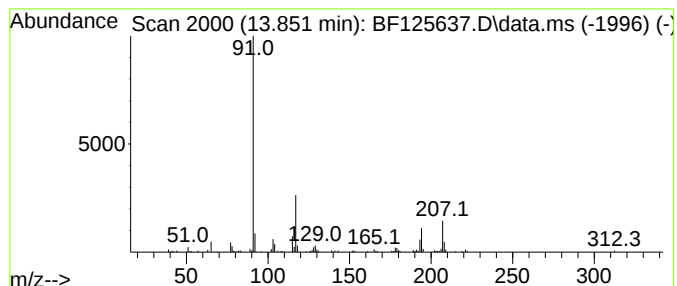
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.53 ng	143187	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	83
2			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20O5	131758-71-9	43
3			Carbonic acid, monoamide, N-benz...	207	C12H17NO2	1000451-48-5	27
4			Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	25
5			DL-Phenylalanine, N-glycyl-	222	C11H14N2O3	000721-66-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

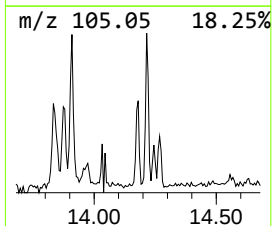
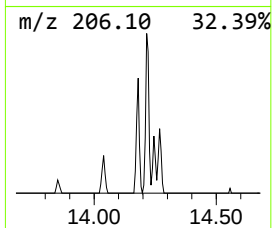
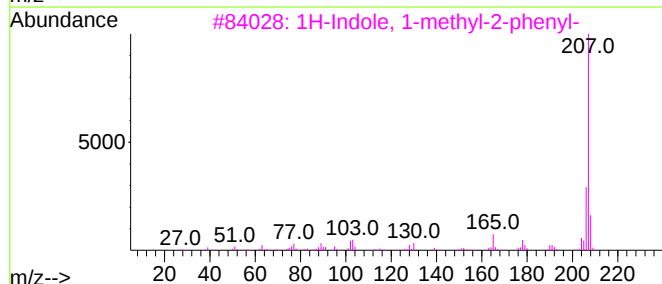
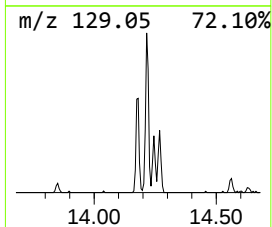
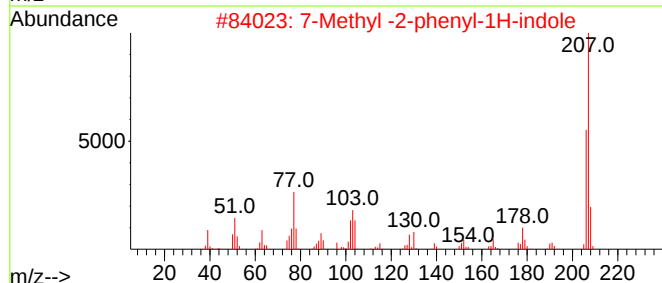
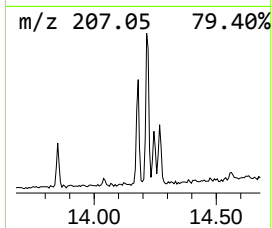
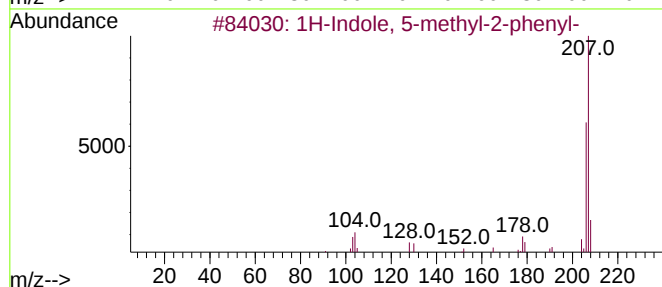
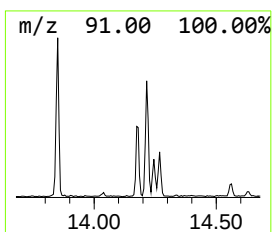
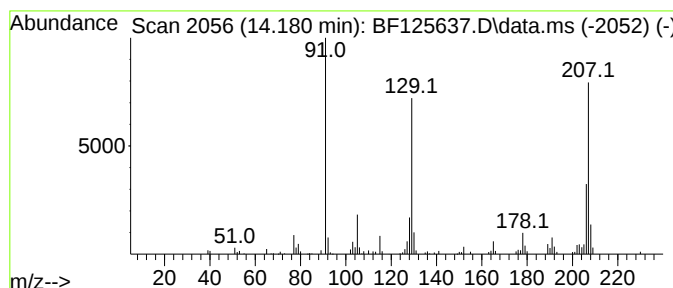
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1H-Indole, 5-methyl-2-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	2.44 ng	137610	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	60
2			7-Methyl -2-phenyl-1H-indole	207	C15H13N	059541-82-1	58
3			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	55
4			1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	53
5			Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

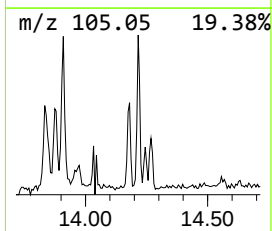
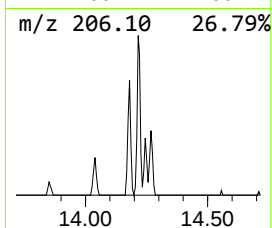
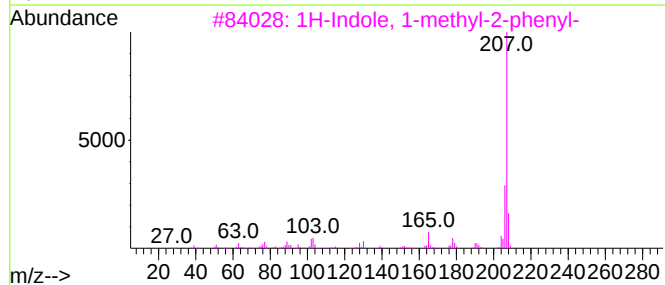
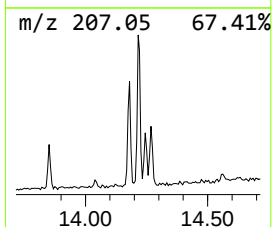
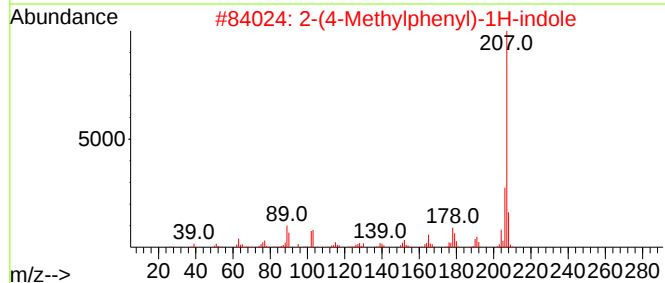
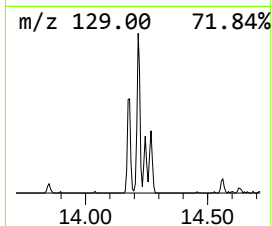
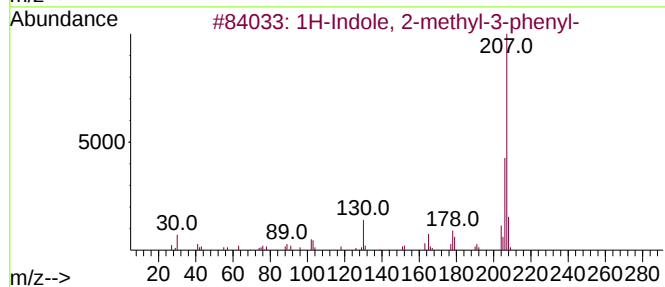
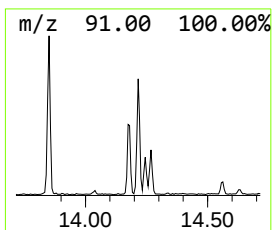
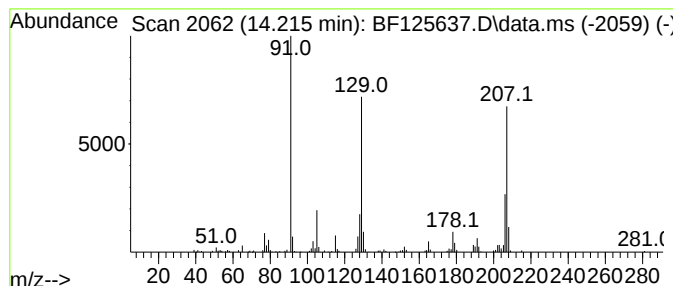
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1H-Indole, 2-methyl-3-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.215	3.94 ng	222475	Chrysene-d12	14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	50
2		2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	42
3		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	41
4		7-Methyl -2-phenyl-1H-indole	207	C15H13N	059541-82-1	35
5		1-benzylindole	207	C15H13N	1000334-31-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

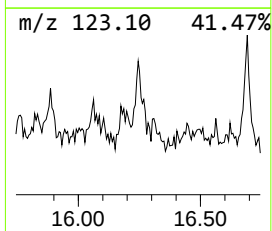
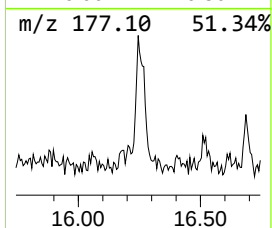
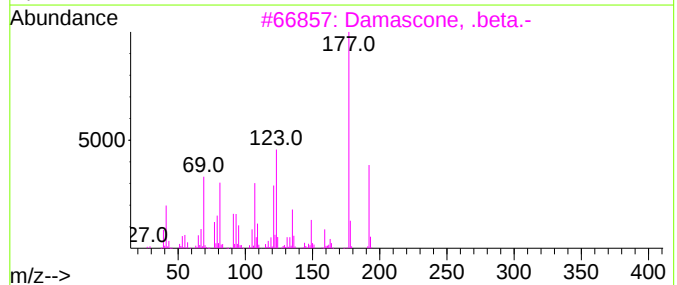
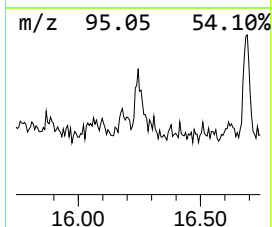
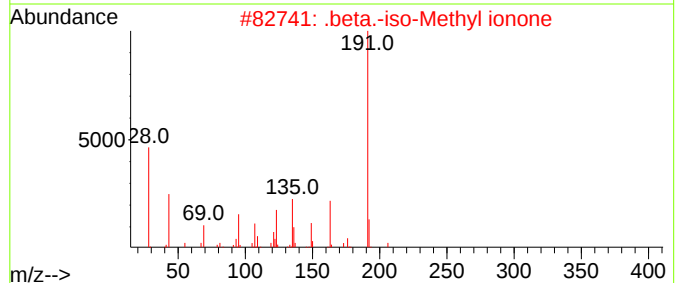
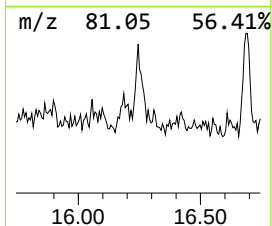
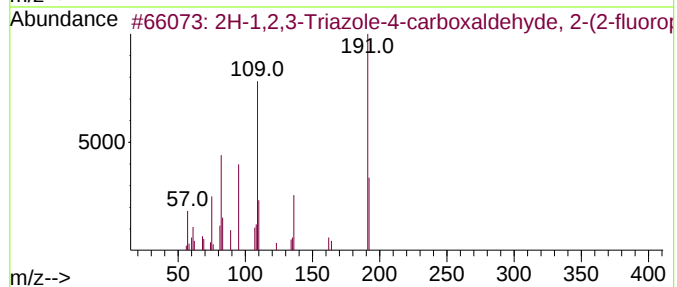
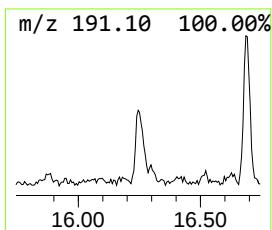
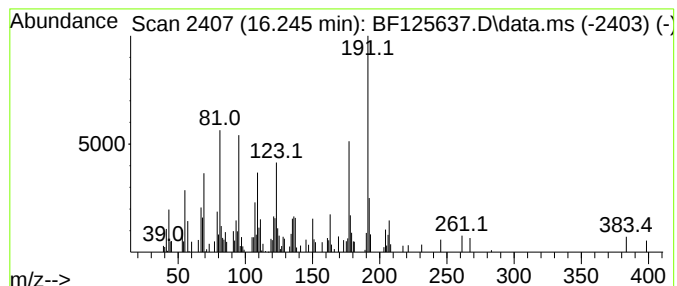
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.245 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	2.17 ng	132409	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	45		
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38		
3	Damascone, .beta.-	192	C13H20O	023726-91-2	27		
4	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	27		
5	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	035044-68-9	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

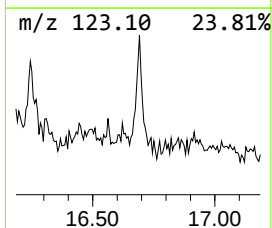
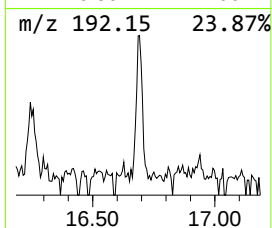
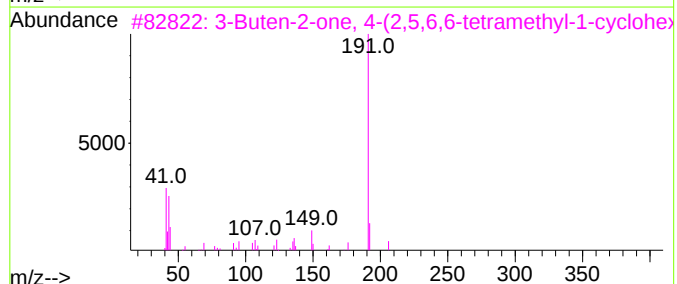
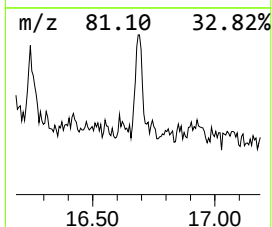
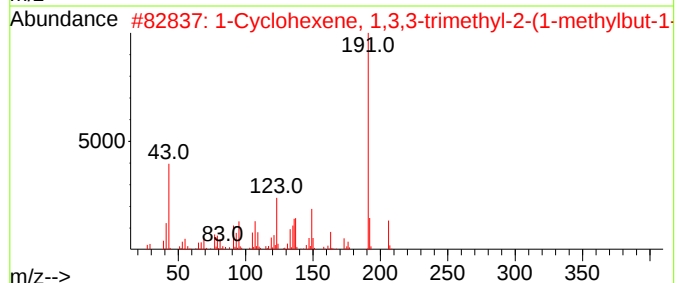
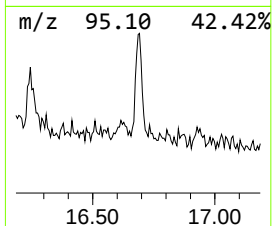
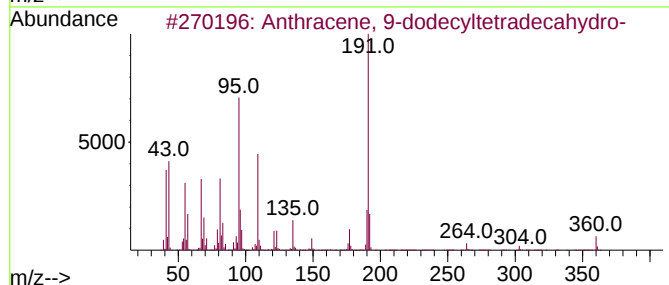
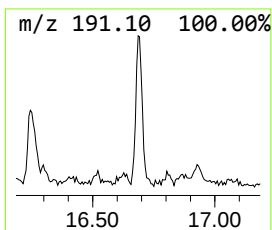
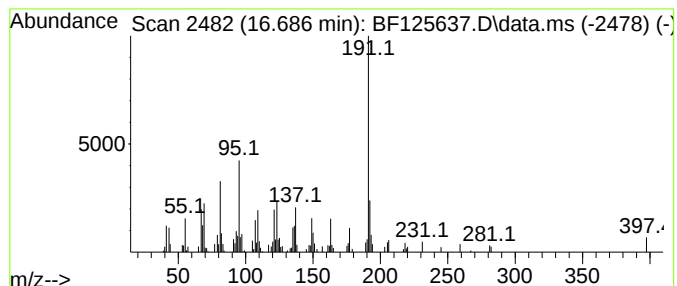
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.686 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.686	3.07 ng	187573	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-dodecyltetradeca...	360	C26H48	055401-75-7	40
2			1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
3			3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	35
4			Anthracene, 9-butyltetradeca...	248	C18H32	055133-89-6	35
5			5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125637.D
Acq On : 24 Sep 2021 23:56
Operator : JU/CG
Sample : M3916-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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
Butane, 2-metho...	2.216	28.1	ng	1755770	1	6.886	1248080	20.0
3-Hexen-2-one	4.504	10.6	ng	663399	1	6.886	1248080	20.0
2-Pentanone, 4-...	5.116	4.3	ng	269626	1	6.886	1248080	20.0
Cyclohexane, 1,...	13.851	2.5	ng	143187	5	14.039	1130180	20.0
1H-Indole, 5-me...	14.180	2.4	ng	137610	5	14.039	1130180	20.0
1H-Indole, 2-me...	14.215	3.9	ng	222475	5	14.039	1130180	20.0
unknown16.245	16.245	2.2	ng	132409	6	15.515	1221980	20.0
unknown16.686	16.686	3.1	ng	187573	6	15.515	1221980	20.0