

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
 Data File : BF127016.D
 Acq On : 22 Feb 2022 18:50
 Operator : CG\JU
 Sample : N1626-15
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CC-A8

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.699	233	240	248	rVB	506217	793862	2.44%	1.553%
2	4.634	377	399	401	rBV	8169100	32564998	100.00%	63.724%
3	5.199	481	495	498	rBV	3244714	8338457	25.61%	16.317%
4	6.916	784	787	791	rBV	564726	422272	1.30%	0.826%
5	7.240	838	842	845	rBV	1116997	923093	2.83%	1.806%
6	7.481	878	883	886	rBV	1530166	1292215	3.97%	2.529%
7	8.198	1001	1005	1008	rBV	717573	559309	1.72%	1.094%
8	9.275	1182	1188	1191	rBV	2889197	2292899	7.04%	4.487%
9	9.957	1300	1304	1307	rBV	740455	576701	1.77%	1.129%
10	10.986	1475	1479	1482	rVB	455557	337557	1.04%	0.661%
11	11.445	1554	1557	1560	rBV	605041	508810	1.56%	0.996%
12	13.033	1823	1827	1830	rVB	1976486	1564411	4.80%	3.061%
13	14.845	2132	2135	2151	rVB	393509	586378	1.80%	1.147%
14	15.592	2258	2262	2269	rVB	255489	341909	1.05%	0.669%

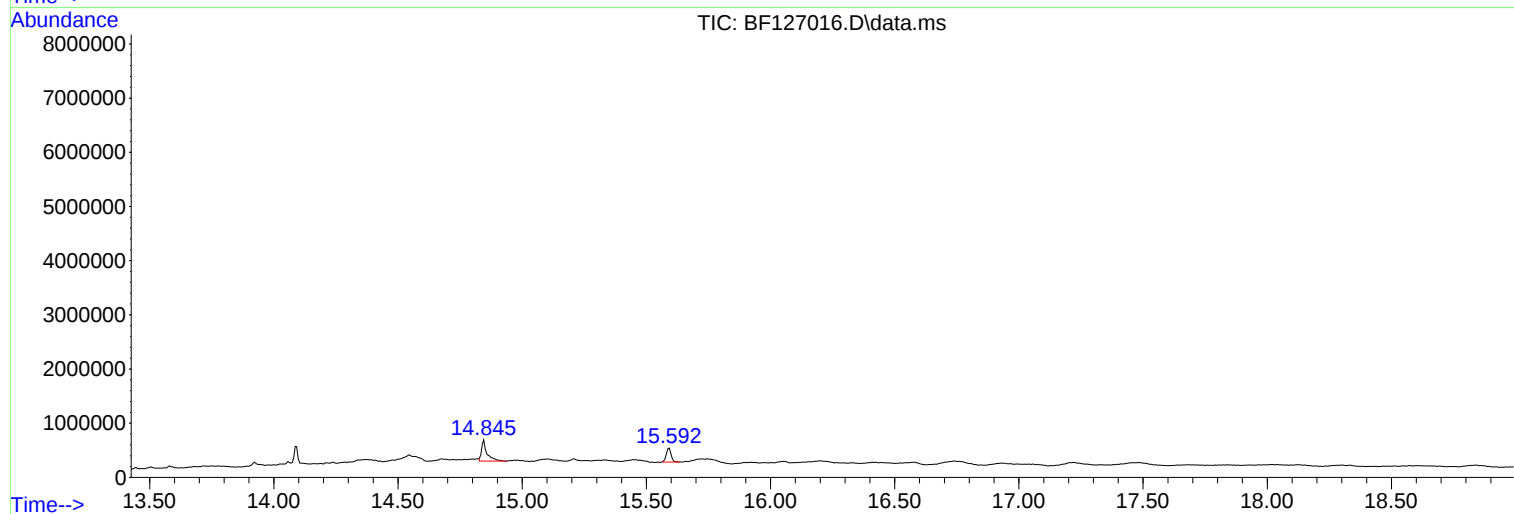
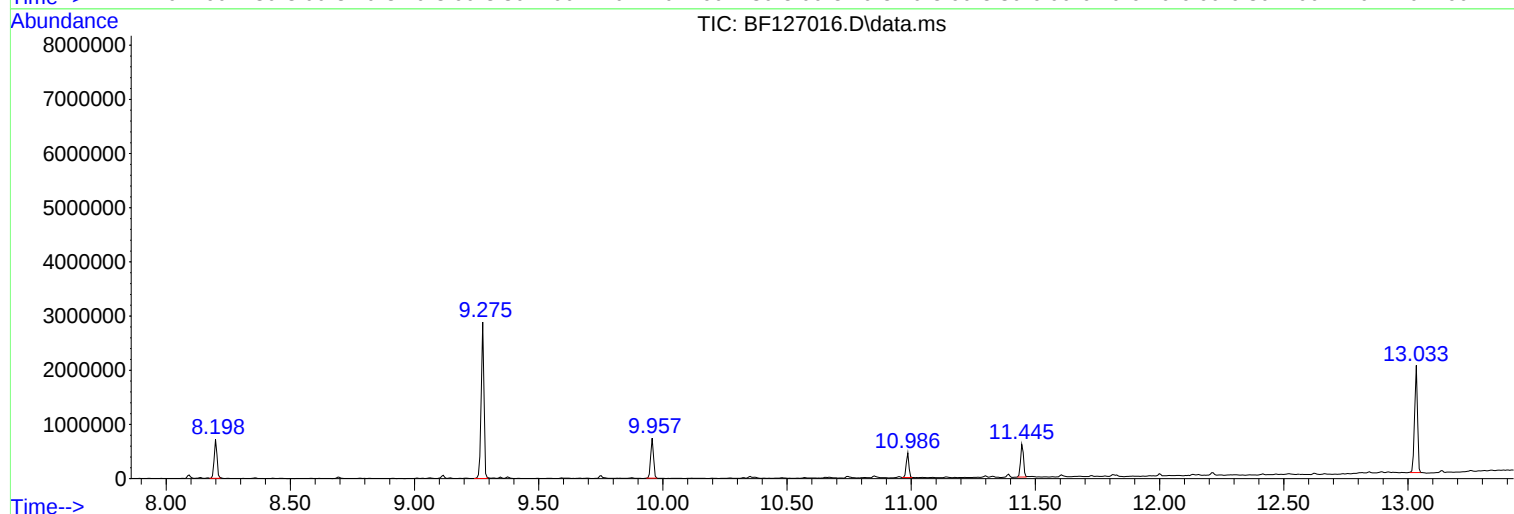
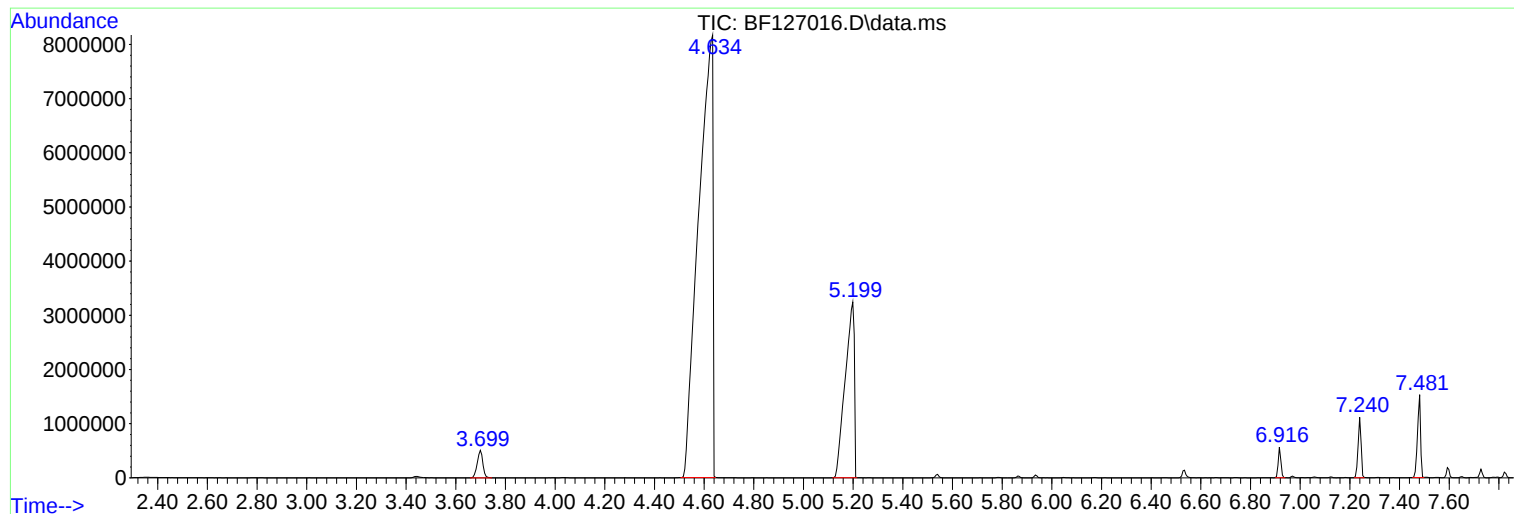
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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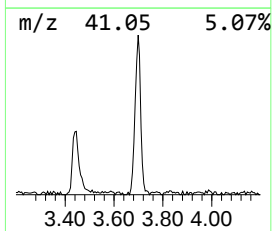
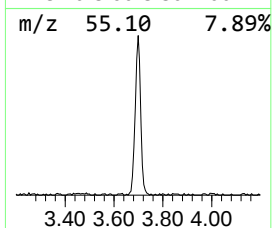
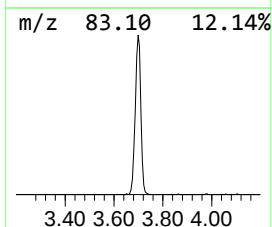
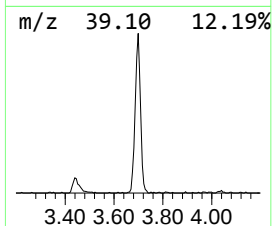
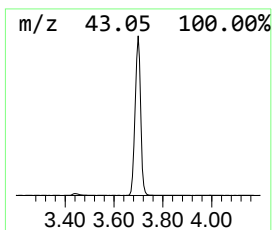
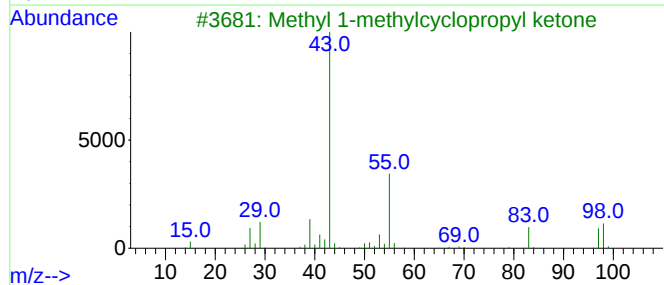
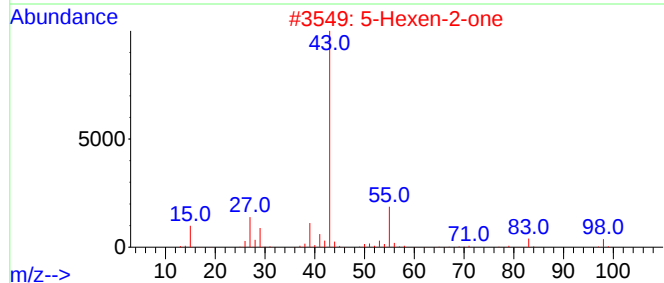
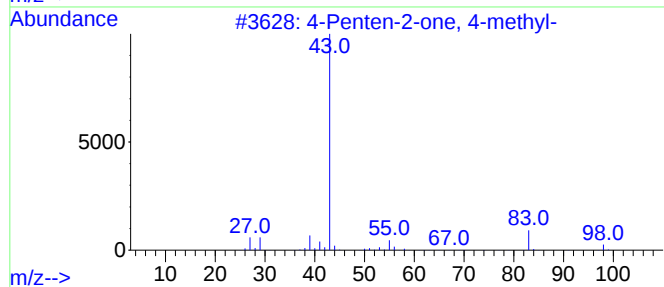
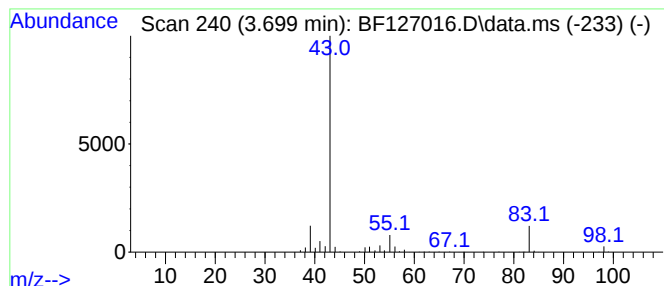
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.699	37.60 ng	793862	1,4-Dichlorobenzene-d4	6.916

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	47
3		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
4		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5		Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	12



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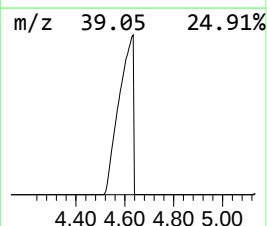
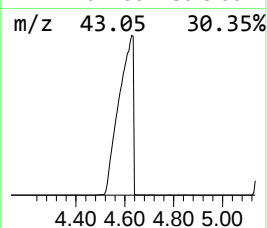
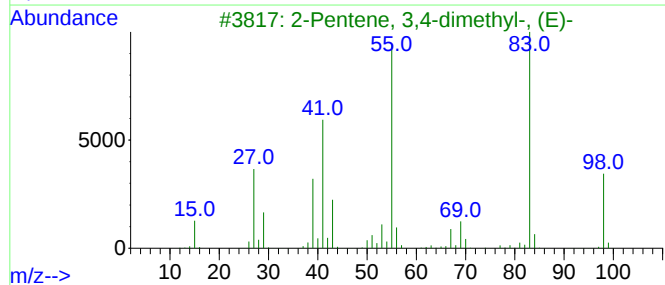
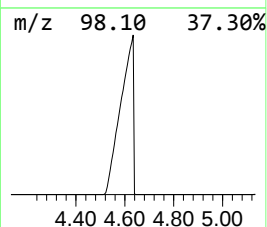
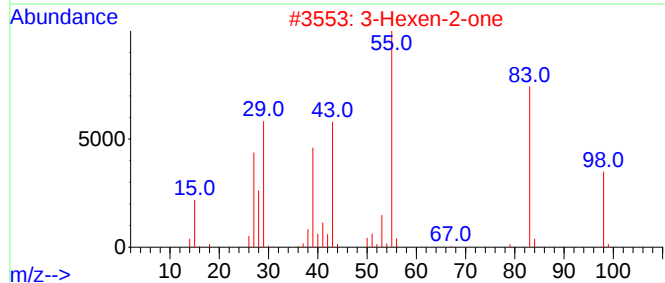
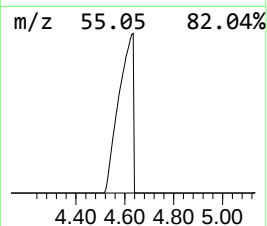
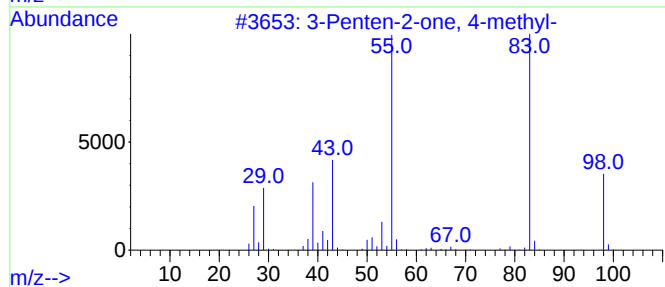
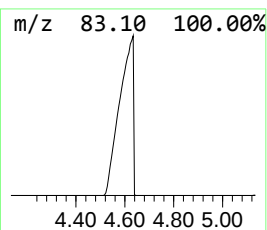
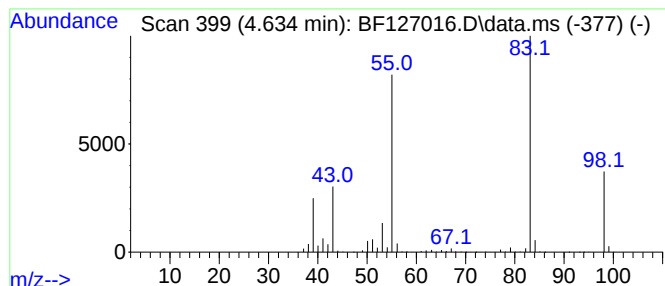
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.634	1542.37 ng	32565000	1,4-Dichlorobenzene-d4	6.916

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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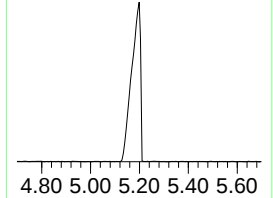
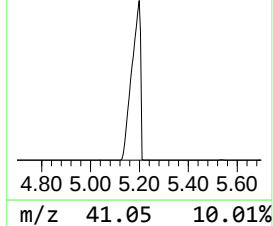
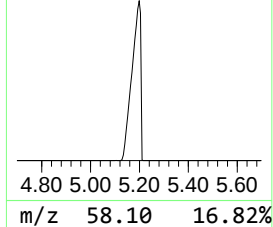
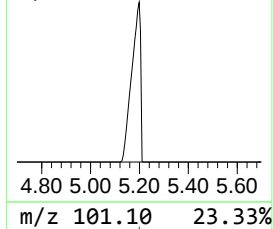
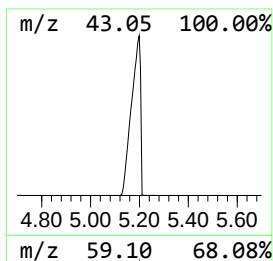
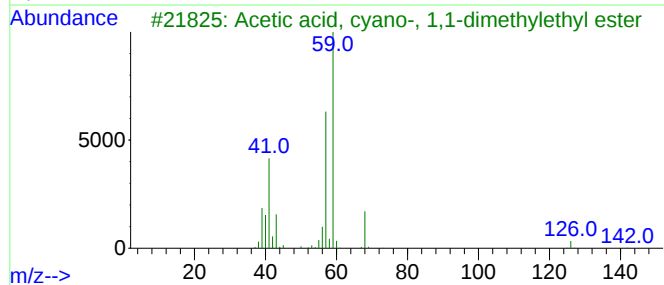
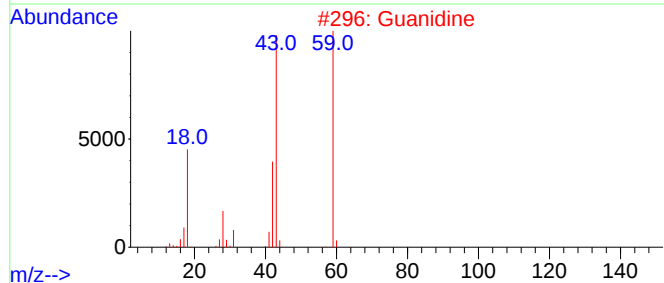
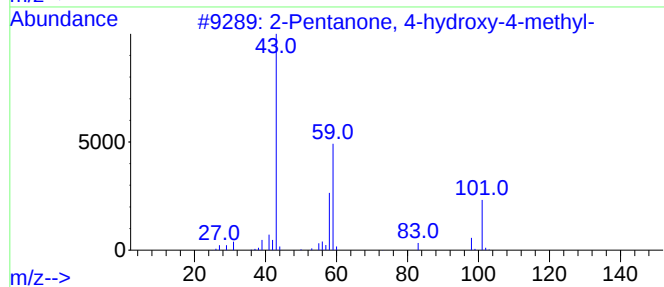
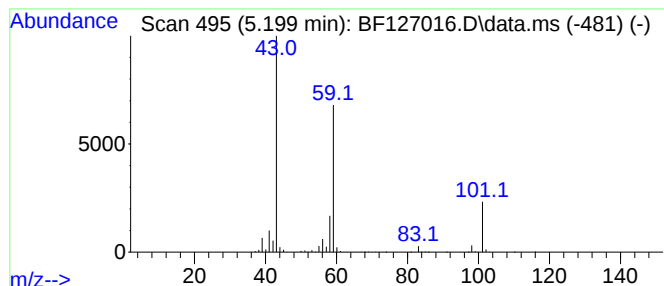
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.199	394.93 ng	8338460	1,4-Dichlorobenzene-d4	6.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	10



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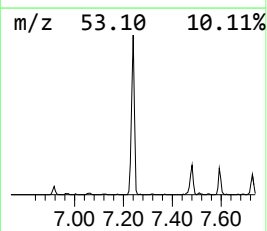
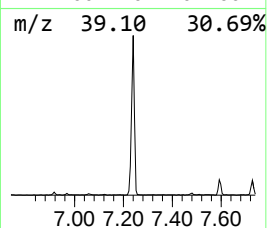
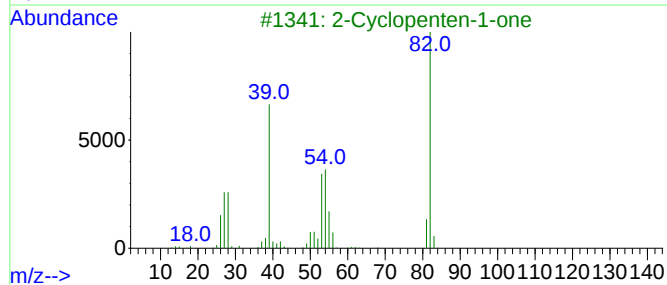
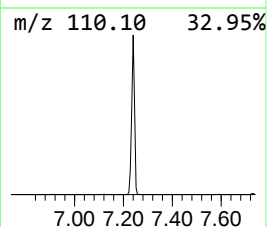
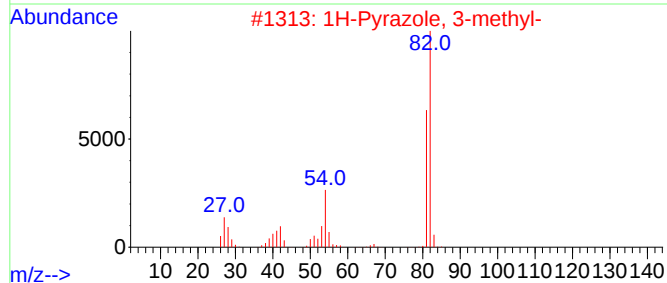
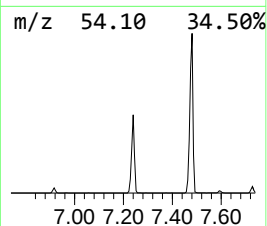
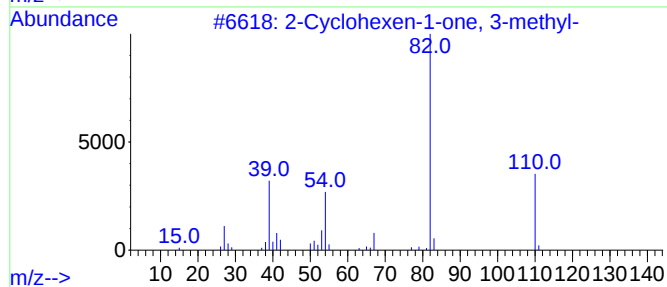
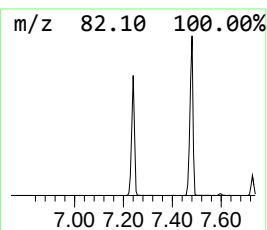
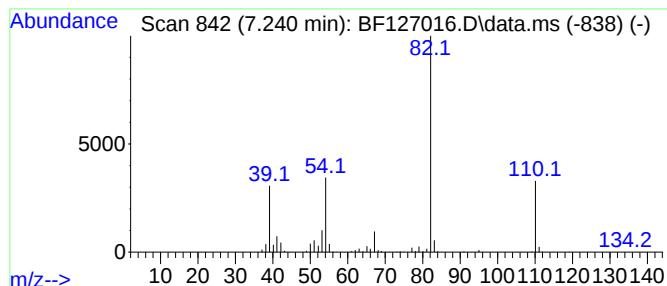
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Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.240	43.72 ng	923093	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	94
2			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	59
3			2-Cyclopenten-1-one	82	C5H6O	000930-30-3	50
4			Betazole	111	C5H9N3	000105-20-4	49
5			2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	43



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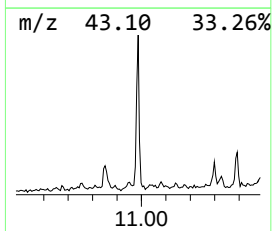
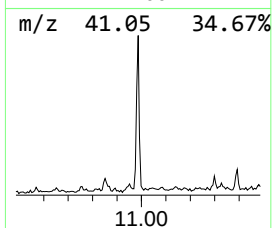
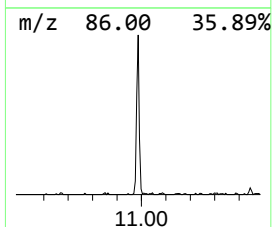
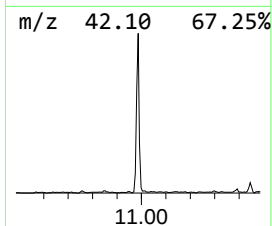
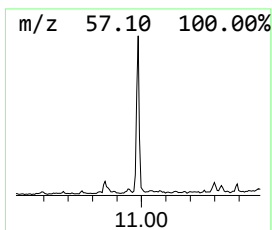
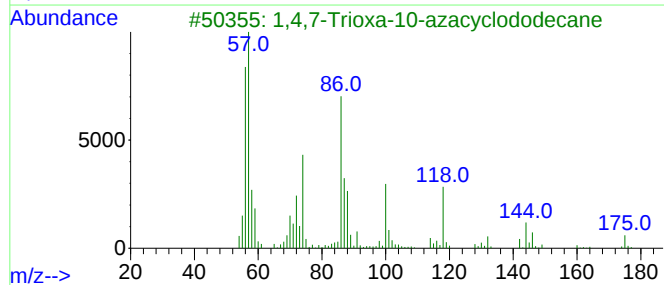
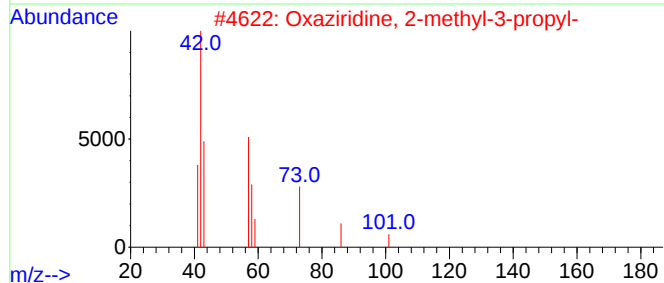
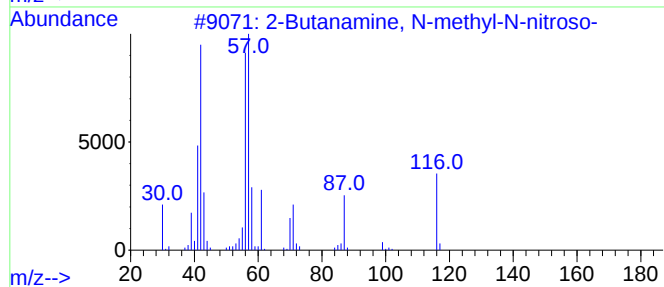
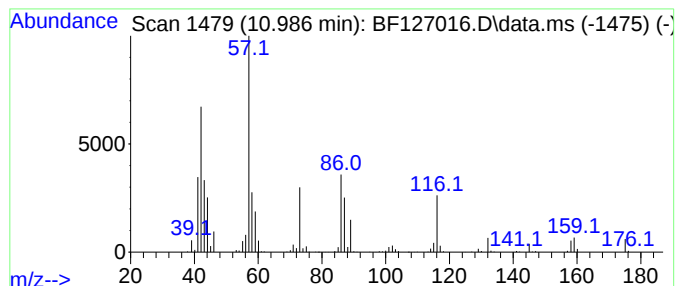
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Butanamine, N-methyl-N-ni... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.986	13.27 ng	337557	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanamine, N-methyl-N-nitroso-	116	C5H12N2O	035606-37-2	50
2			Oxaziridine, 2-methyl-3-propyl-	101	C5H11NO	058751-77-2	43
3			1,4,7-Trioxa-10-azacyclododecane	175	C8H17NO3	041775-76-2	23
4			N1-(4-hydroxybutyl)-N3-methylgua...	205	C8H19N3O3	1010188-13-5	23
5			1,3-Dibutoxy-2-propanol	204	C11H24O3	002216-77-5	12



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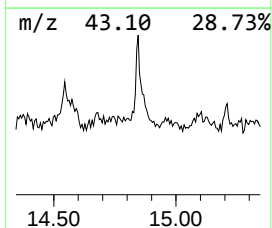
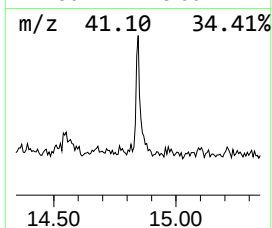
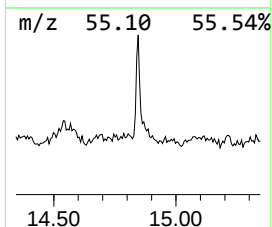
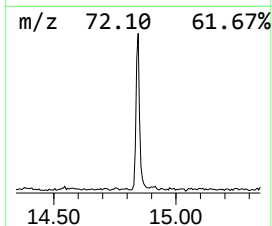
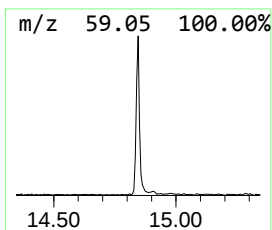
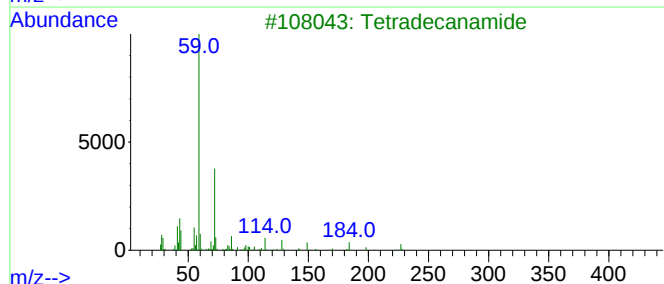
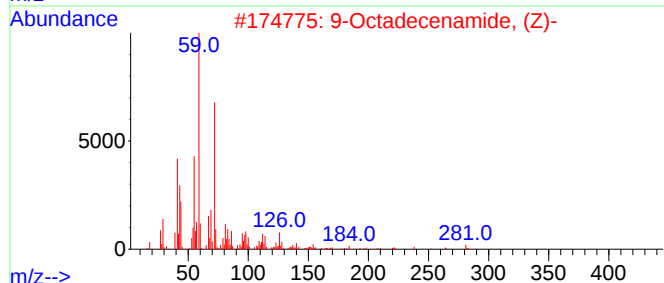
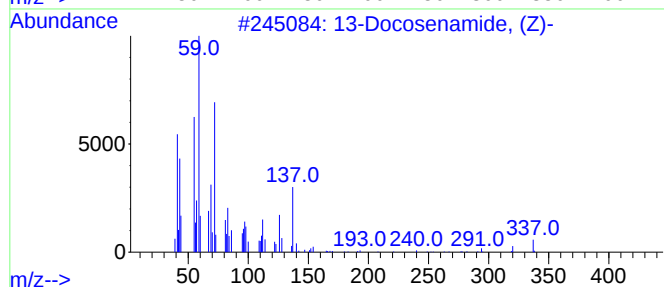
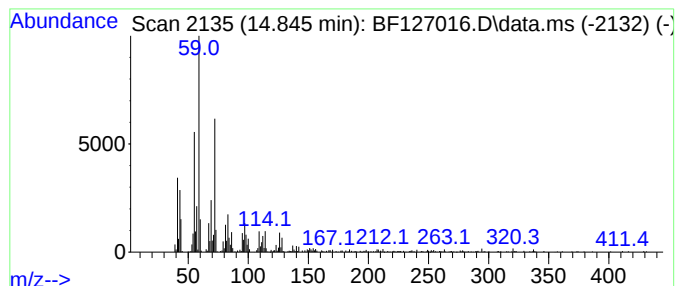
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	34.30 ng	586378	Perylene-d12	15.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3			Tetradecanamide	227	C14H29NO	000638-58-4	64
4			Palmitoleamide	253	C16H31NO	106010-22-4	64
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022222\
Data File : BF127016.D
Acq On : 22 Feb 2022 18:50
Operator : CG\JU
Sample : N1626-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CC-A8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
4-Penten-2-one,...	3.699	37.6	ng	793862	1	6.916	422272	20.0
3-Penten-2-one,...	4.634	1542.4	ng	32565000	1	6.916	422272	20.0
2-Pentanone, 4-...	5.199	394.9	ng	8338460	1	6.916	422272	20.0
2-Cyclohexen-1-...	7.240	43.7	ng	923093	1	6.916	422272	20.0
2-Butanamine, N...	10.986	13.3	ng	337557	4	11.445	508810	20.0
13-Docosenamide...	14.845	34.3	ng	586378	6	15.592	341909	20.0