

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010423\
 Data File : BF131899.D
 Acq On : 04 Jan 2023 15:09
 Operator : CG\JU
 Sample : 01004-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CONTAINMENT-STONES

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-BF122422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	8	12	21	rVB	38584	49452	2.34%	0.345%
2	5.016	493	498	509	rVB	567673	709844	33.61%	4.959%
3	5.428	563	568	571	rBV	1816947	1691127	80.08%	11.814%
4	5.681	608	611	615	rBV	99119	83831	3.97%	0.586%
5	6.445	736	741	744	rBV	1690552	1742330	82.50%	12.172%
6	6.810	799	803	807	rBV	568000	457747	21.68%	3.198%
7	7.381	895	900	903	rBV	1213855	1141144	54.04%	7.972%
8	8.098	1016	1022	1026	rBV	617366	577110	27.33%	4.032%
9	8.692	1117	1123	1126	rBV	22144	21416	1.01%	0.150%
10	9.186	1201	1207	1210	rBV	2157349	2111854	100.00%	14.753%
11	9.257	1215	1219	1222	rBV	66696	63631	3.01%	0.445%
12	9.581	1269	1274	1276	rBV4	30451	43857	2.08%	0.306%
13	9.675	1288	1290	1295	rBV5	32491	44188	2.09%	0.309%
14	9.722	1295	1298	1301	rBV4	49173	66688	3.16%	0.466%
15	9.769	1303	1306	1308	rBV2	38304	35920	1.70%	0.251%
16	9.792	1308	1310	1311	rBV	42810	30285	1.43%	0.212%
17	9.863	1319	1322	1326	rVB	782645	651026	30.83%	4.548%
18	10.657	1454	1457	1462	rBV	1185629	1147032	54.31%	8.013%
19	10.980	1510	1512	1515	rBV	180865	182670	8.65%	1.276%
20	11.363	1574	1577	1580	rBV	726593	586025	27.75%	4.094%
21	12.398	1751	1753	1758	rVB	315559	335096	15.87%	2.341%
22	12.951	1843	1847	1850	rVB	1751947	1496093	70.84%	10.452%
23	13.857	1998	2001	2013	rVB6	79379	196941	9.33%	1.376%
24	14.010	2023	2027	2035	rVB	448833	390974	18.51%	2.731%
25	14.863	2169	2172	2177	rVB3	23517	29453	1.39%	0.206%
26	15.486	2273	2278	2287	rVB	339908	428772	20.30%	2.995%

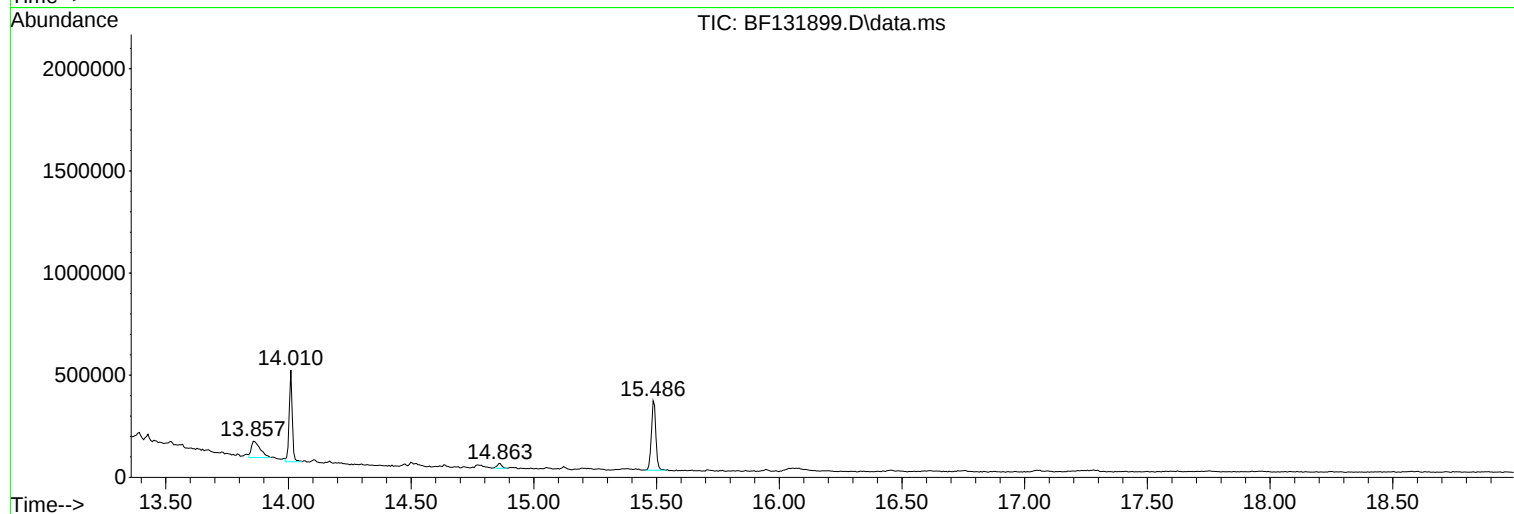
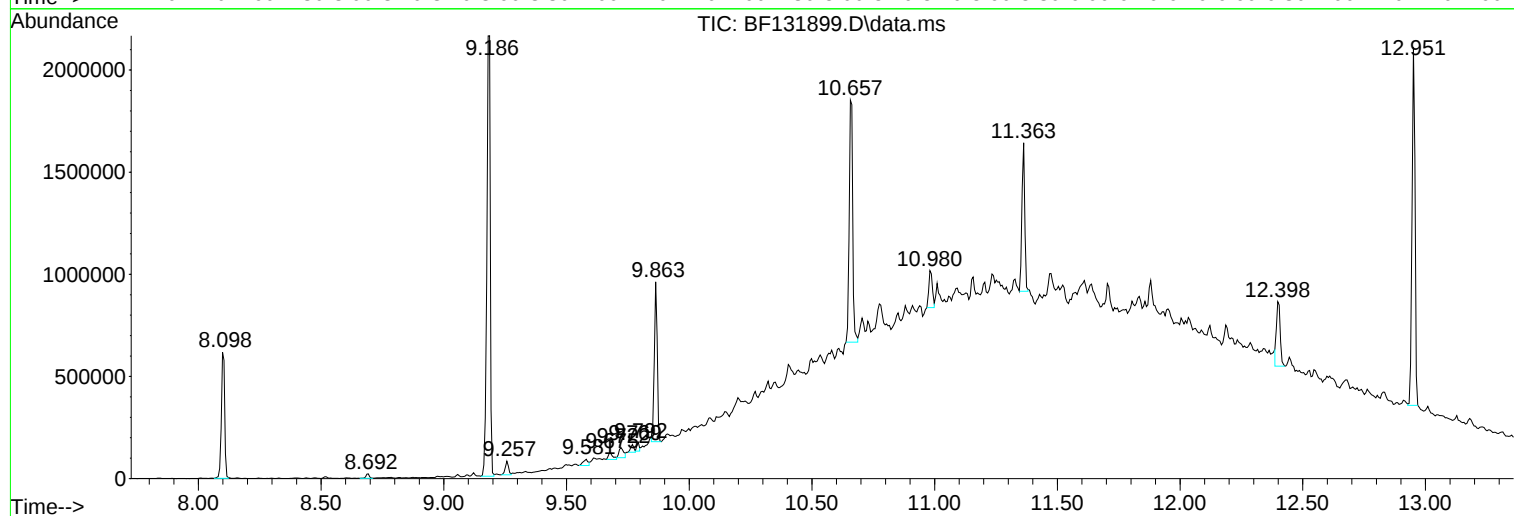
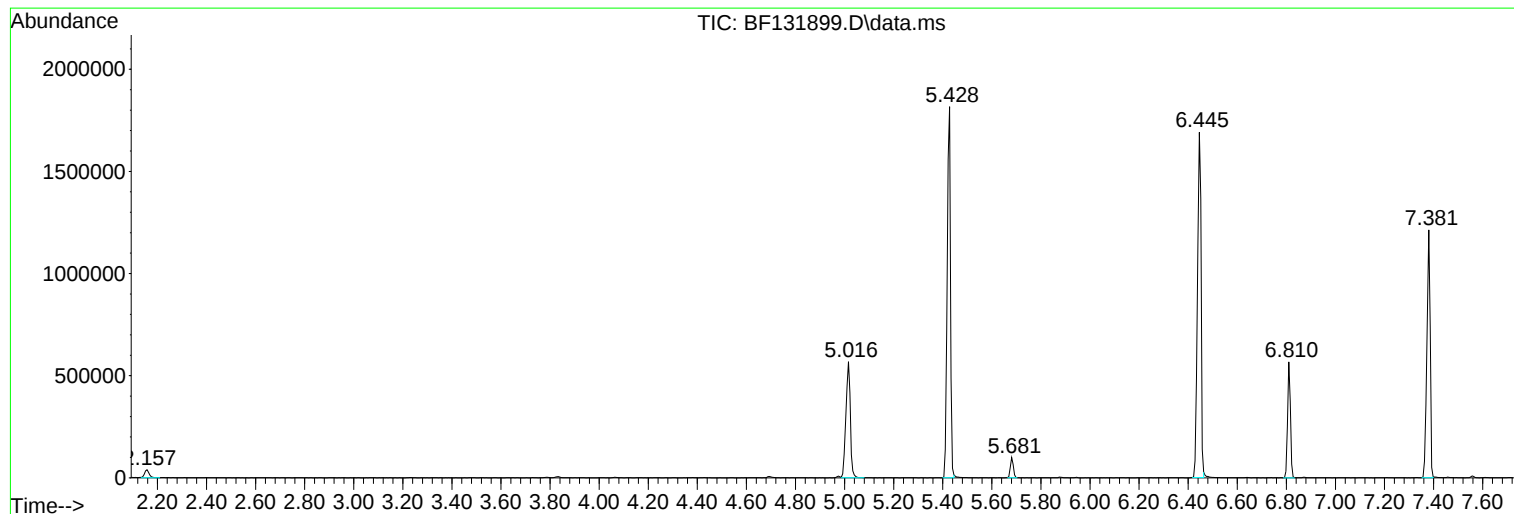
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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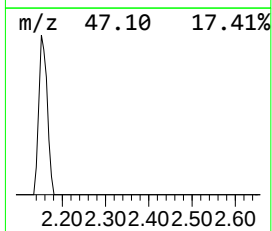
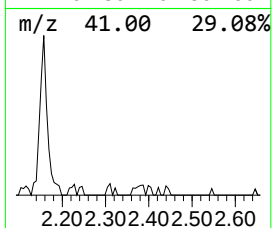
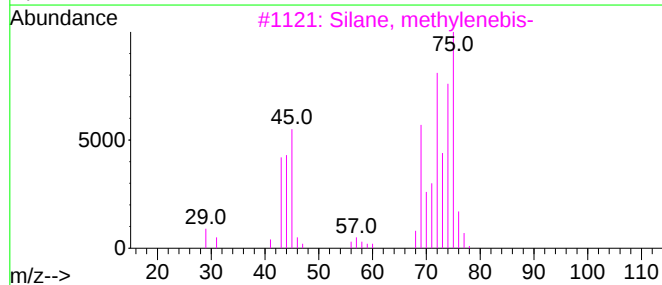
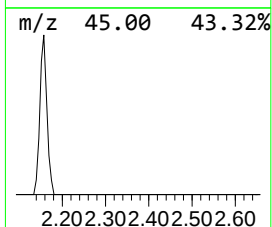
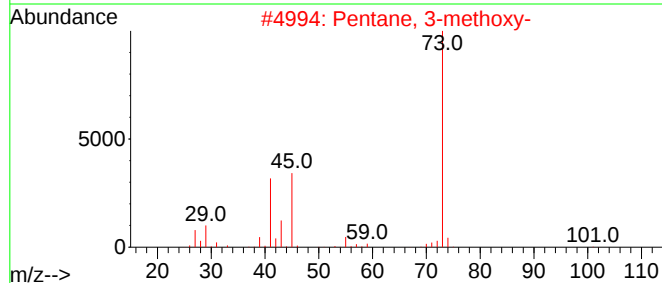
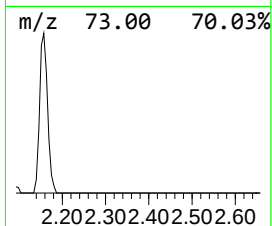
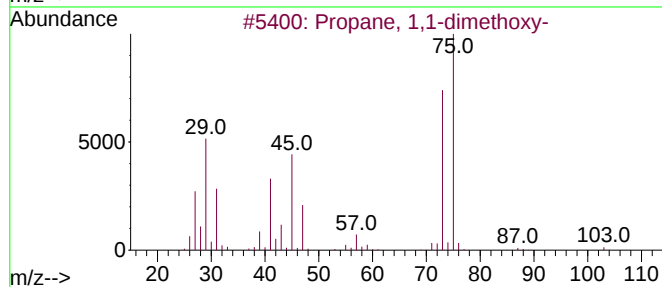
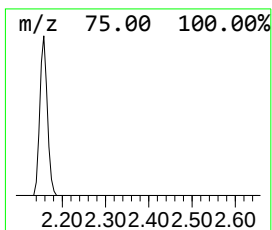
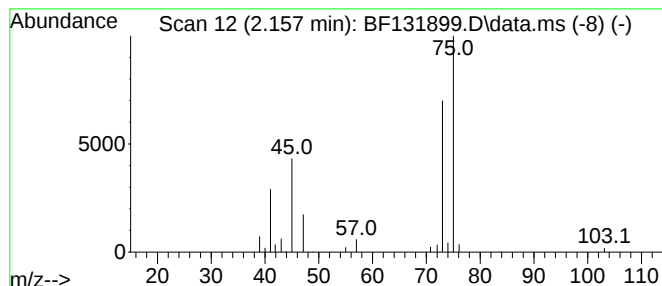
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	2.16 ng	49452	1,4-Dichlorobenzene-d4	6.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3			Silane, methylenebis-	76	CH8Si2	001759-88-2	9
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5			Disilane, pentamethyl(pentafluor...	298	C11H15F5Si2	033558-55-3	9



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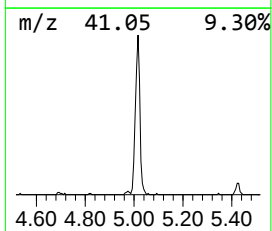
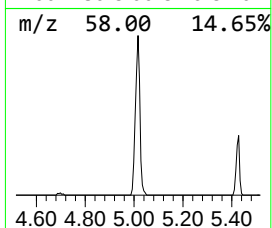
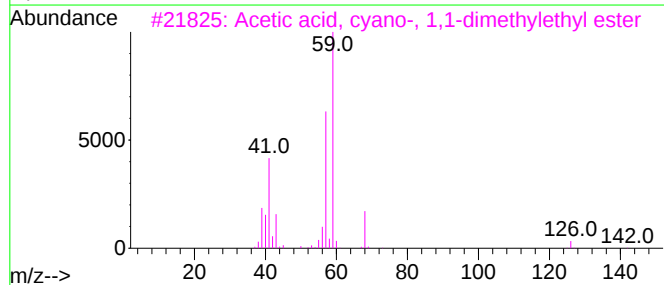
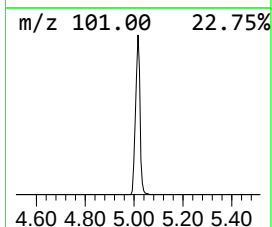
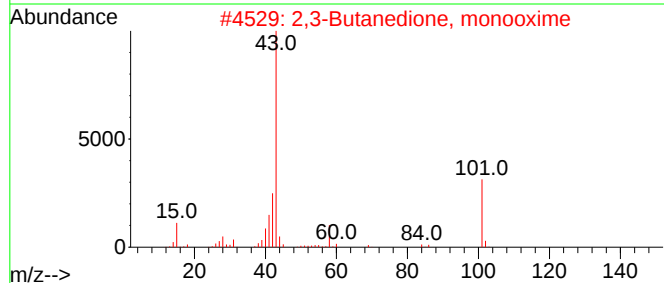
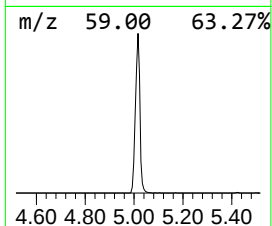
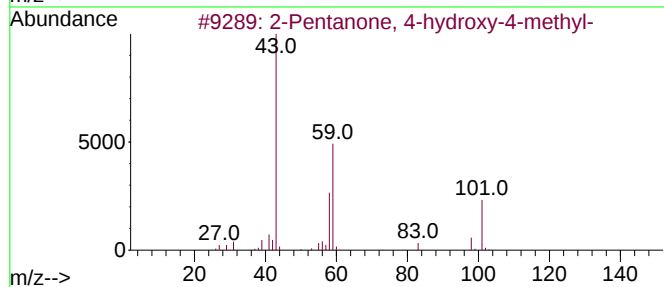
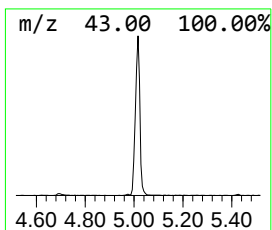
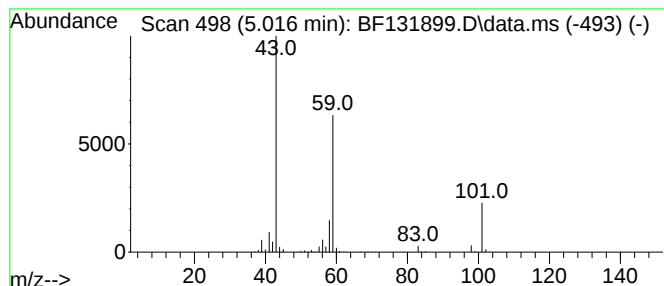
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.016	31.01 ng	709844	1,4-Dichlorobenzene-d4			6.810
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	25
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	Butane, 1-ethoxy-		102	C6H14O	000628-81-9	9



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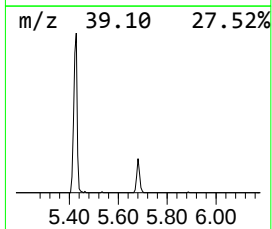
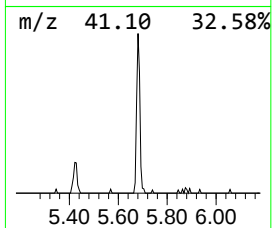
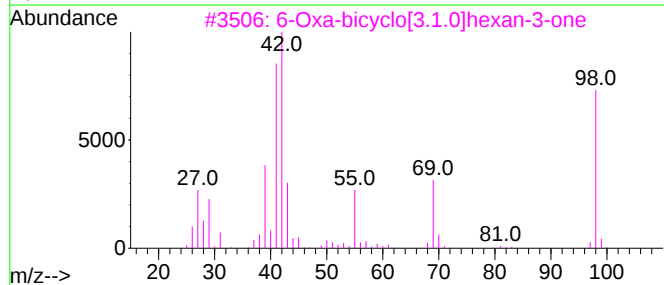
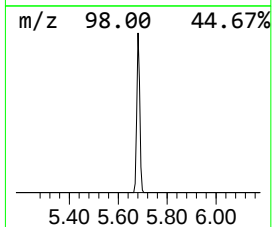
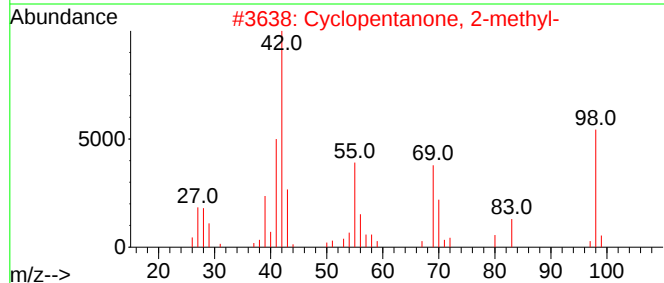
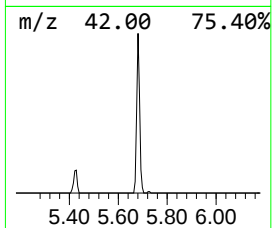
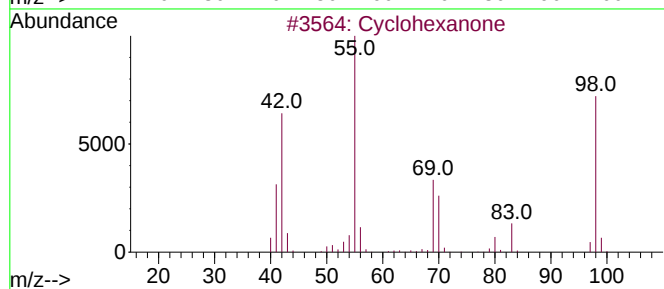
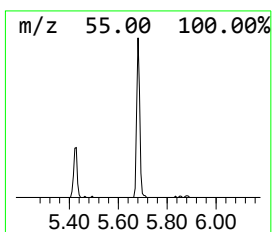
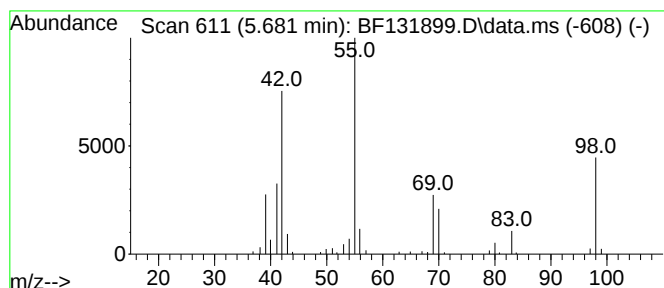
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.681	3.66 ng	83831	1,4-Dichlorobenzene-d4	6.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	91
2			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	86
3			6-Oxa-bicyclo[3.1.0]hexan-3-one	98	C5H6O2	074017-10-0	53
4			2-Pentene, (E)-	70	C5H10	000646-04-8	43
5			1-Pentene	70	C5H10	000109-67-1	43



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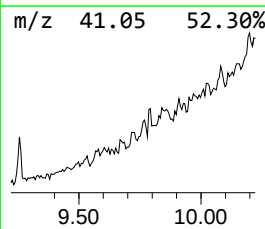
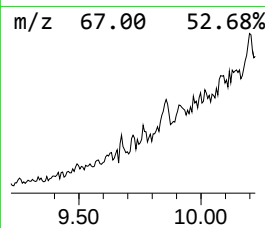
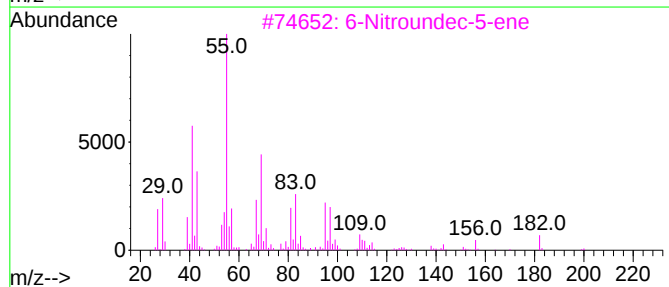
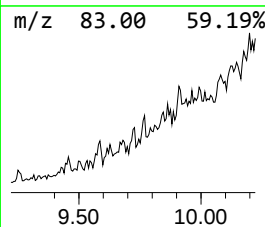
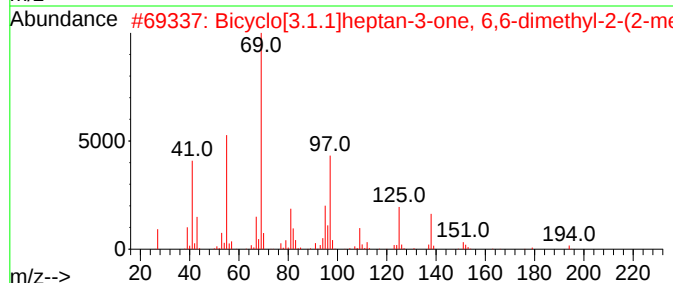
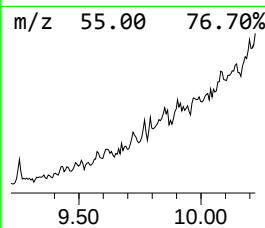
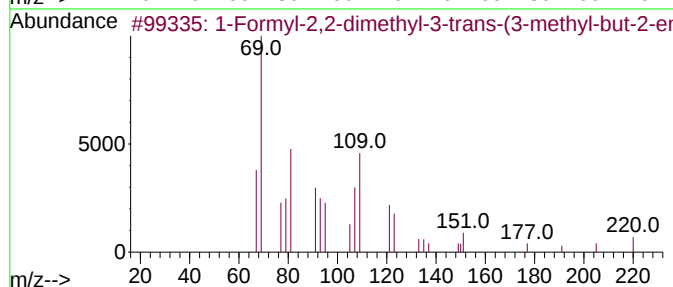
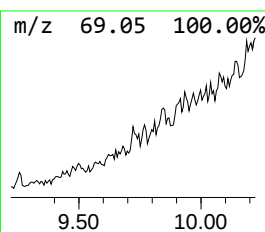
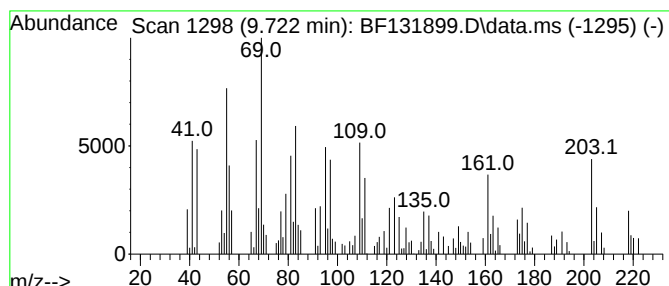
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Peak Number 4 unknown9.722 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.722	2.05 ng	66688	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	41
2			Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	38
3			6-Nitroundec-5-ene	199	C11H21NO2	1000192-40-3	38
4			Bicyclo[3.1.1]heptan-3-one, 2,6-...	152	C10H16O	015358-88-0	27
5			2-n-Hexylthiolane, S,S-dioxide	204	C10H20O2S	071053-04-8	25



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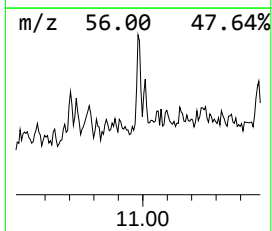
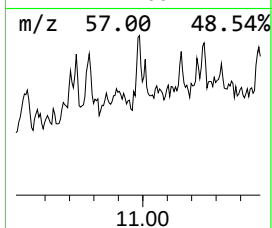
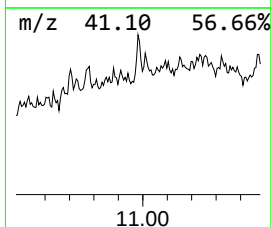
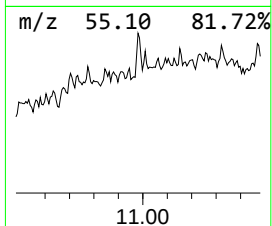
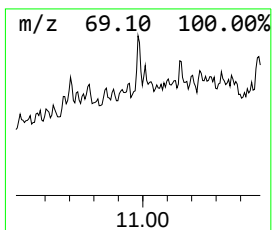
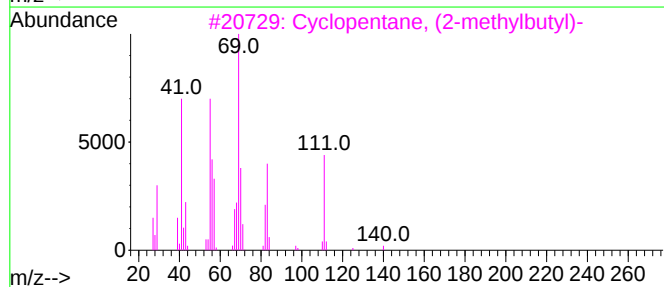
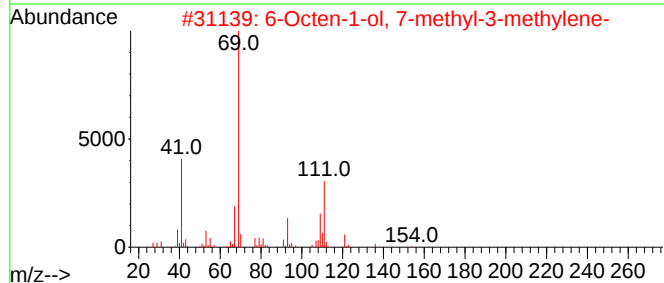
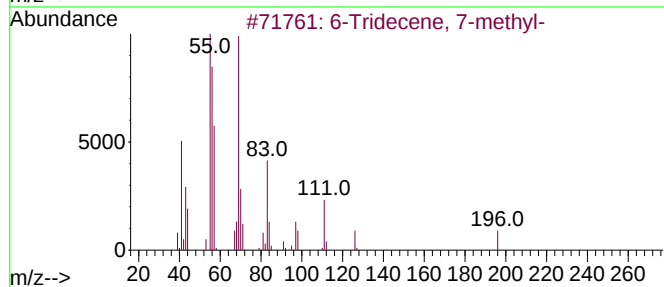
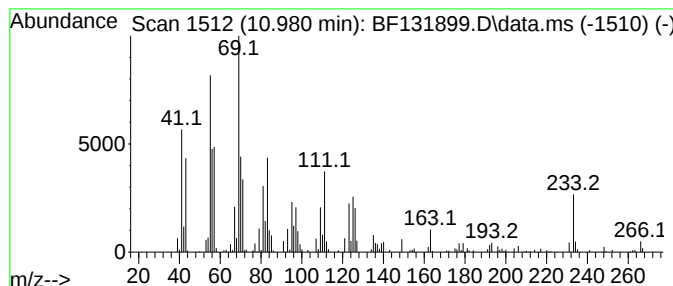
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 6-Tridecene, 7-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.980	6.23 ng	182670	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Tridecene, 7-methyl-	196	C14H28	024949-42-6	53
2			6-Octen-1-ol, 7-methyl-3-methylene-	154	C10H18O	013066-51-8	46
3			Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	38
4			2-(Acetylmethylene)tetrahydrofuran	126	C7H10O2	112595-65-0	30
5			3-Tridecene, (E)-	182	C13H26	041446-57-5	25



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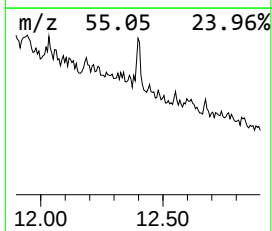
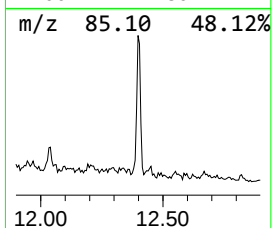
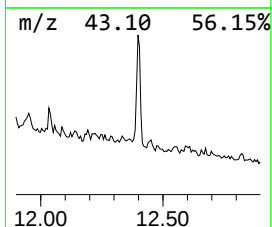
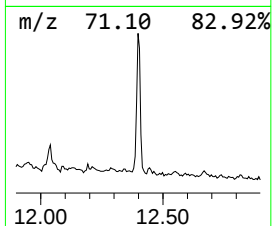
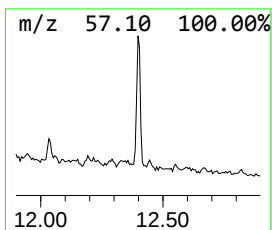
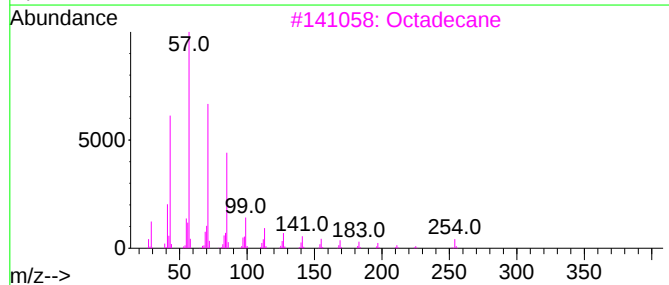
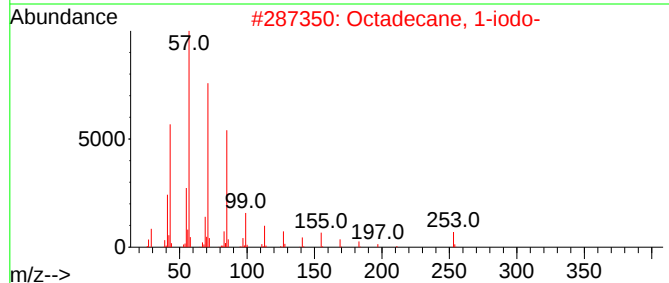
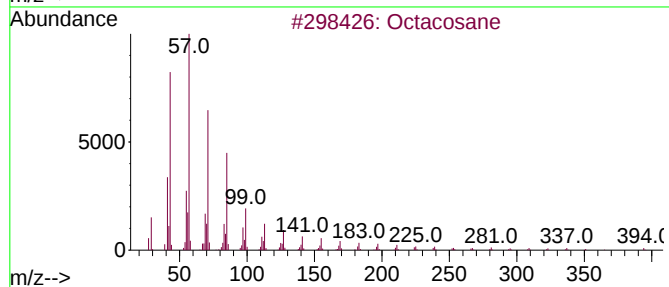
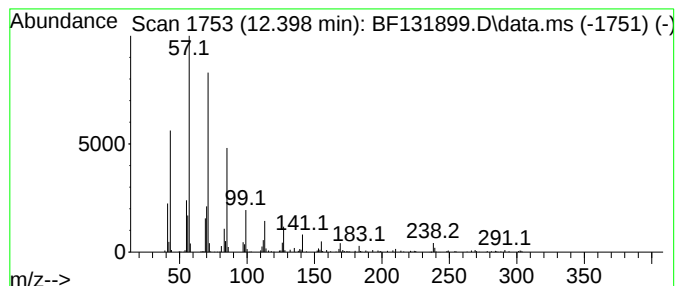
Instrument :
BNA_F
ClientSampleId :
CONTAINMENT-STONES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.398	11.44 ng	335096	Phenanthrene-d10		11.363
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3	Octadecane	254	C18H38	000593-45-3	86
4	Heptacosane	380	C27H56	000593-49-7	86
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010423\
Data File : BF131899.D
Acq On : 04 Jan 2023 15:09
Operator : CG\JU
Sample : 01004-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONTAINMENT-STONES

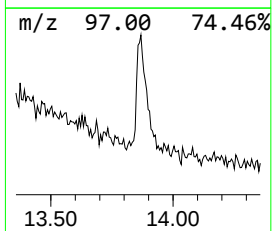
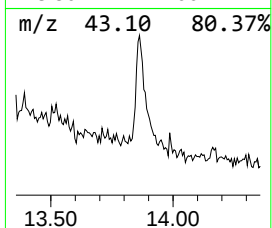
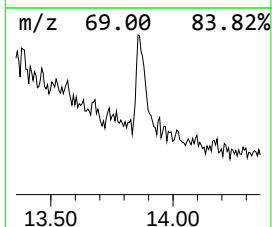
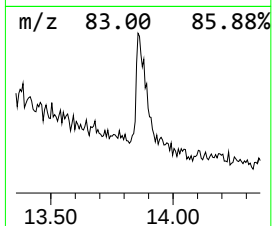
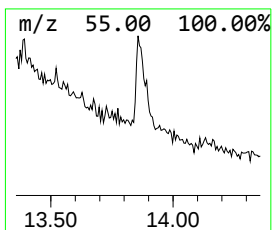
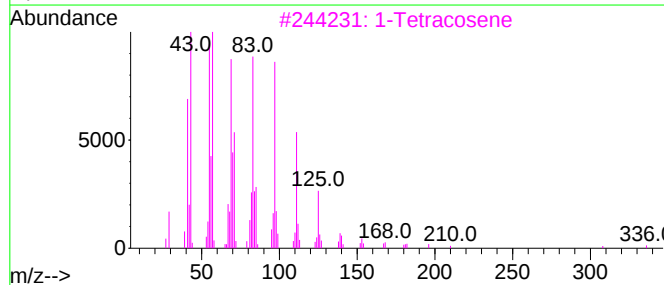
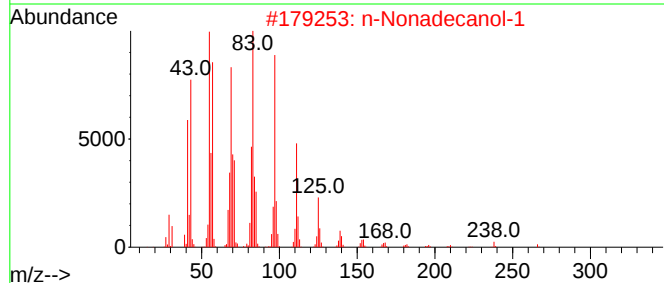
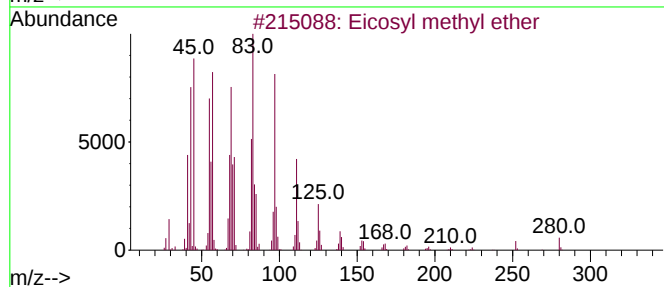
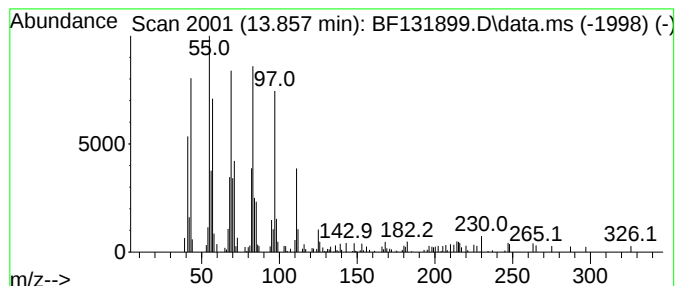
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosyl methyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	10.07 ng	196941	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl methyl ether	312	C21H44O	1000406-29-4	91
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3			1-Tetracosene	336	C24H48	010192-32-2	87
4			Cyclopentadecane	210	C15H30	000295-48-7	87
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010423\
Data File : BF131899.D
Acq On : 04 Jan 2023 15:09
Operator : CG\JU
Sample : 01004-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONTAINMENT-STONES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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
Propane, 1,1-di...	2.157	2.2	ng	49452	1	6.810	457747	20.0
2-Pentanone, 4-...	5.016	31.0	ng	709844	1	6.810	457747	20.0
Cyclohexanone	5.681	3.7	ng	83831	1	6.810	457747	20.0
unknown9.722	9.722	2.0	ng	66688	3	9.863	651026	20.0
6-Tridecene, 7-...	10.980	6.2	ng	182670	4	11.363	586025	20.0
Octacosane	12.398	11.4	ng	335096	4	11.363	586025	20.0
Eicosyl methyl ...	13.857	10.1	ng	196941	5	14.010	390974	20.0