

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060722\
 Data File : BF128714.D
 Acq On : 07 Jun 2022 13:47
 Operator : CG\JU
 Sample : N3189-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220423-AMENDED-COMPOSITE-C

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128714.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.452	186	198	209	rBV	125203	370658	3.80%	1.506%
2	4.722	409	414	421	rVB	64586	104859	1.07%	0.426%
3	5.098	463	478	481	rVB	3557114	9761292	100.00%	39.667%
4	5.493	542	545	553	rBV	303221	274286	2.81%	1.115%
5	6.492	712	715	725	rVB	886618	899139	9.21%	3.654%
6	6.822	767	771	777	rBV	683108	531010	5.44%	2.158%
7	7.392	861	868	871	rBV	1788524	1932256	19.80%	7.852%
8	7.539	889	893	896	rBV	530160	492618	5.05%	2.002%
9	8.104	984	989	993	rBV	786429	680071	6.97%	2.764%
10	9.186	1167	1173	1176	rBV	3205690	2798248	28.67%	11.371%
11	9.863	1284	1288	1291	rVB	973895	777649	7.97%	3.160%
12	10.380	1373	1376	1380	rBV2	143032	128552	1.32%	0.522%
13	10.651	1415	1422	1424	rBV	223575	279892	2.87%	1.137%
14	10.775	1438	1443	1450	rBV3	150128	178530	1.83%	0.725%
15	11.222	1515	1519	1529	rBV2	101042	143222	1.47%	0.582%
16	11.351	1537	1541	1544	rBV	1110344	900885	9.23%	3.661%
17	12.945	1807	1812	1815	rBV	3123436	2864505	29.35%	11.641%
18	13.845	1962	1965	1978	rBV	114984	190544	1.95%	0.774%
19	13.998	1985	1991	1993	rBV	656787	680915	6.98%	2.767%
20	14.092	2002	2007	2013	rBV	156664	163773	1.68%	0.666%
21	15.462	2235	2240	2244	rBV	367996	455009	4.66%	1.849%

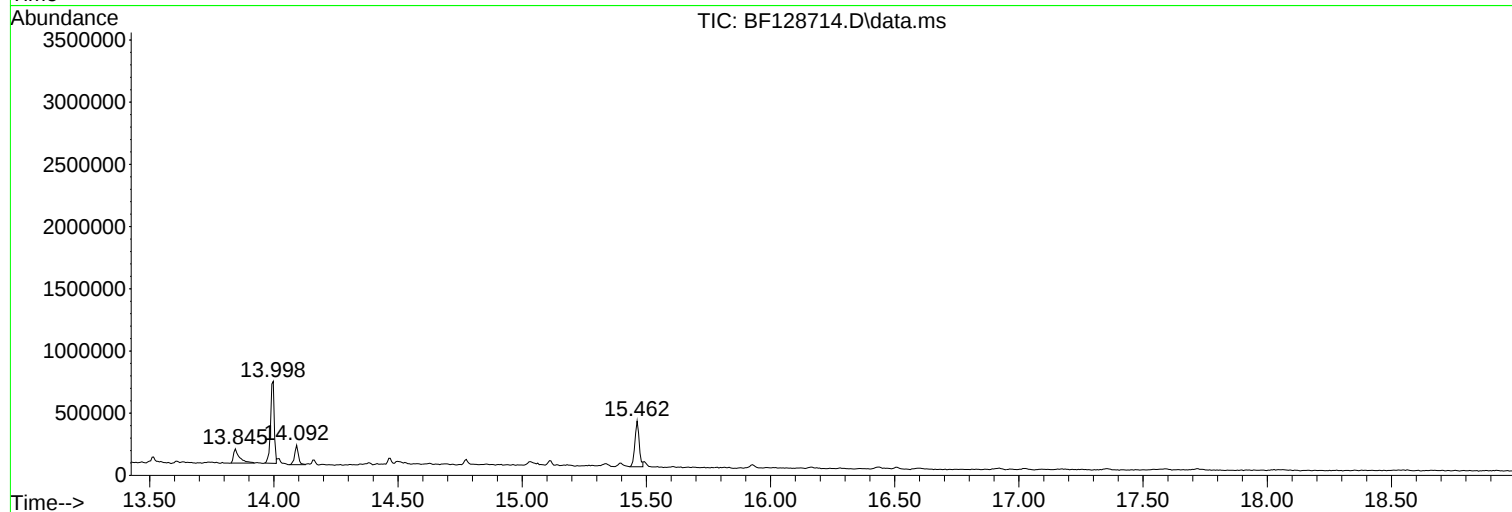
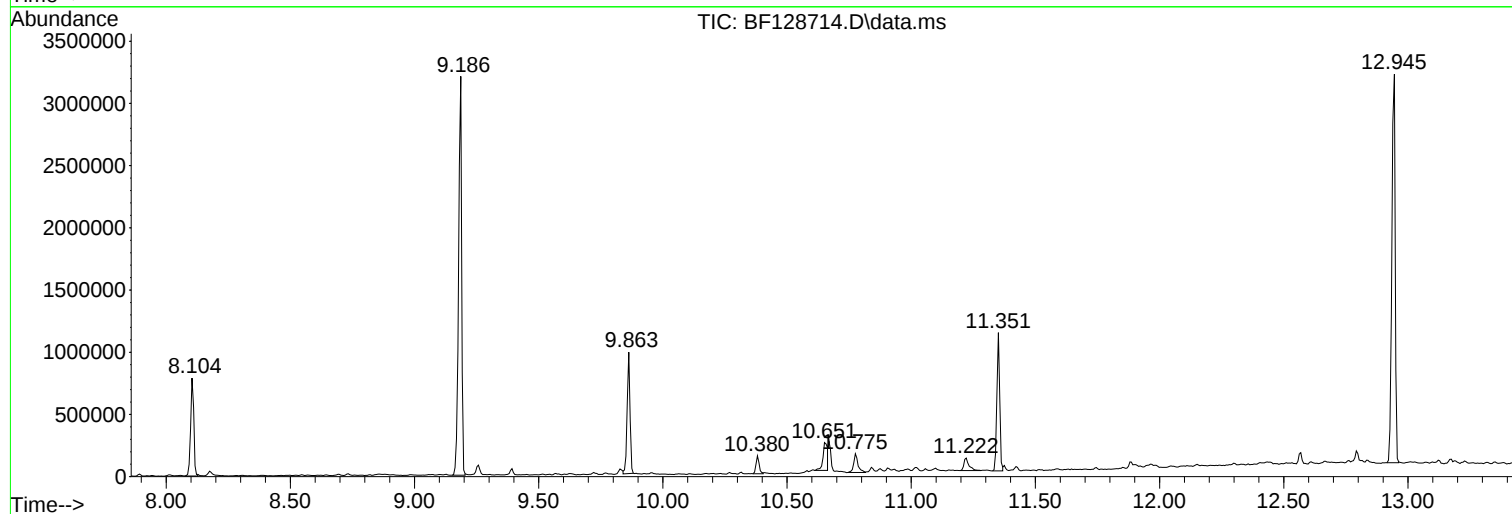
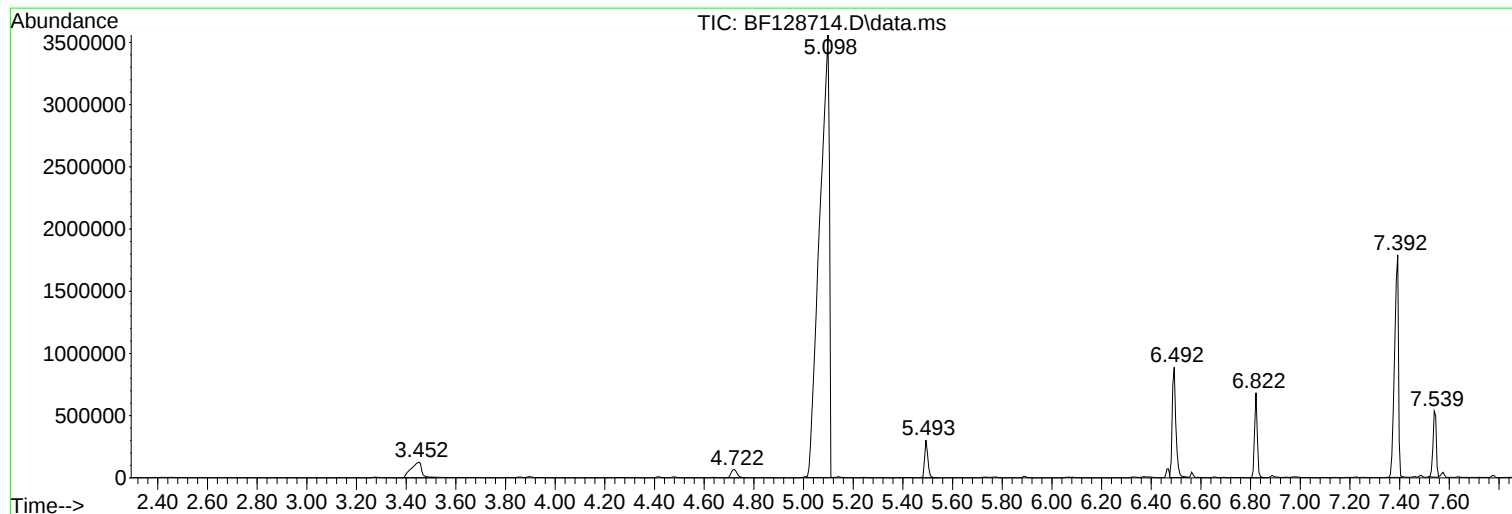
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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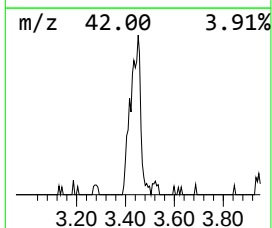
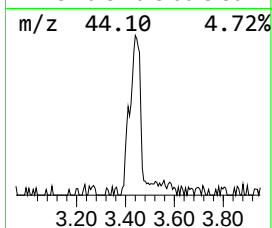
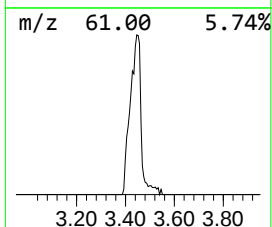
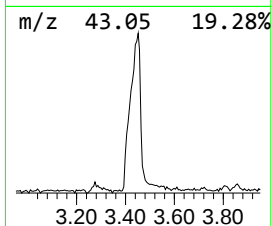
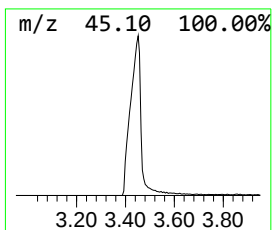
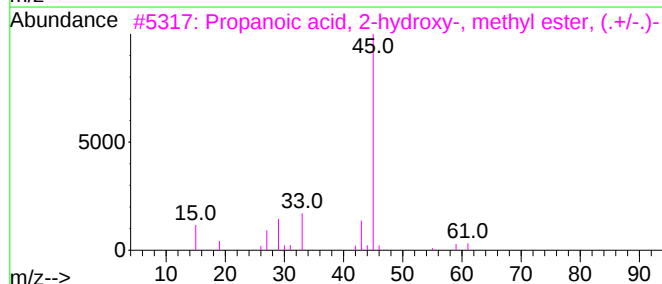
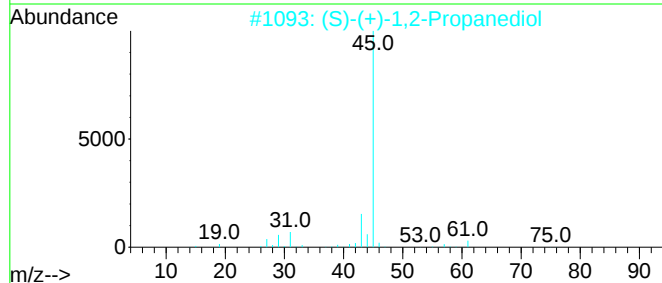
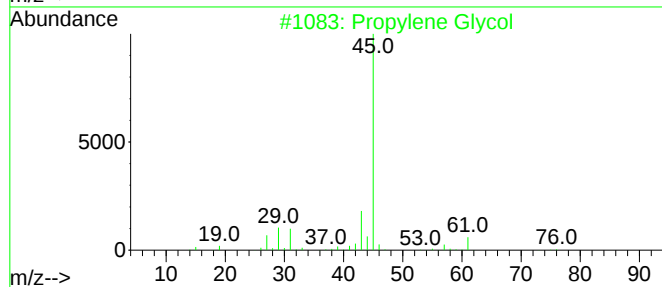
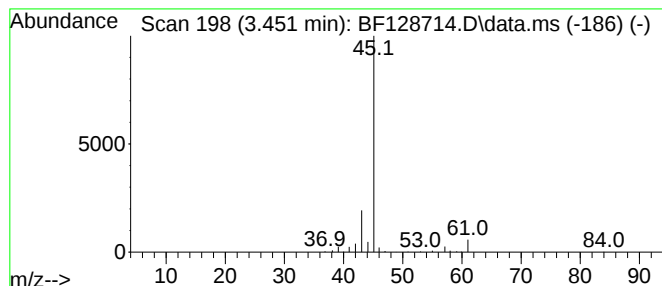
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.451	13.96 ng	370658	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	64
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Formamide	45	CH3NO	000075-12-7	5



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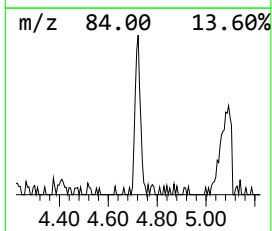
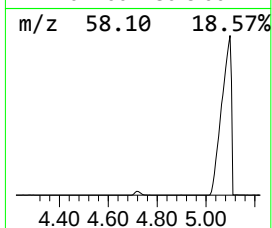
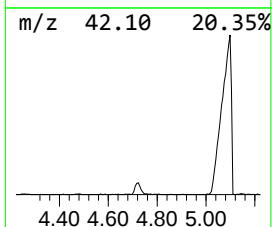
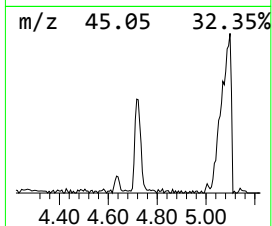
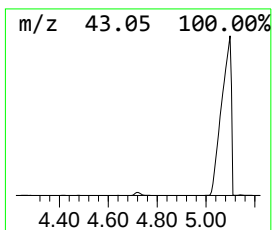
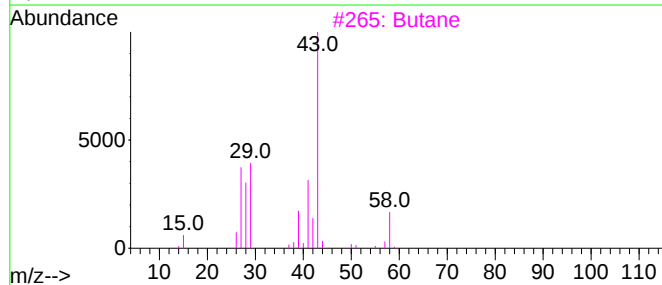
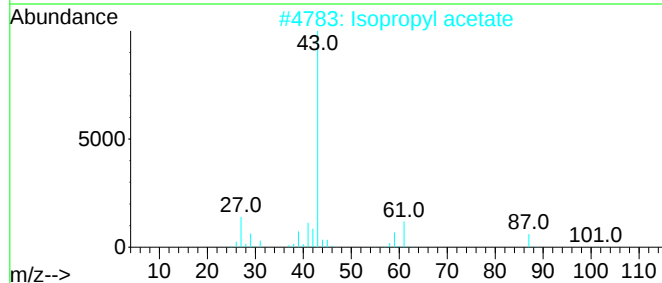
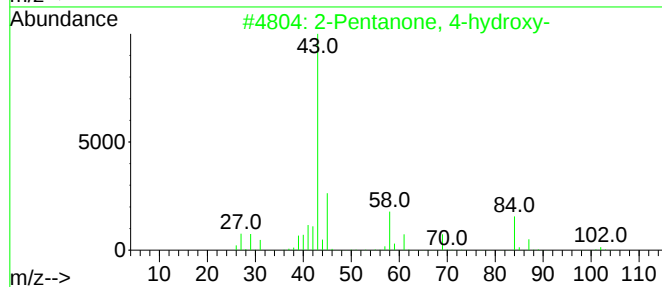
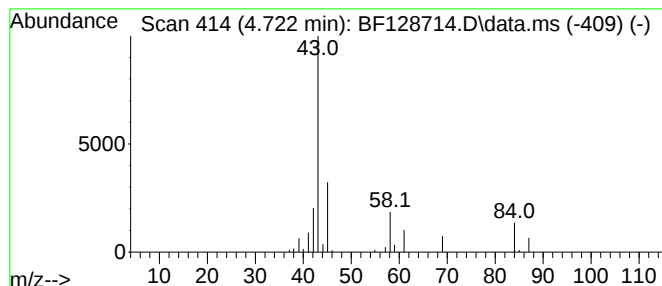
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.722	3.95 ng	104859	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-	102	C5H10O2	004161-60-8	64
2			Isopropyl acetate	102	C5H10O2	000108-21-4	17
3			Butane	58	C4H10	000106-97-8	9
4			Acetone	58	C3H6O	000067-64-1	9
5			Oxirane, 2,3-dimethyl-, trans-	72	C4H8O	021490-63-1	9



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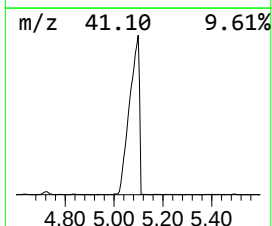
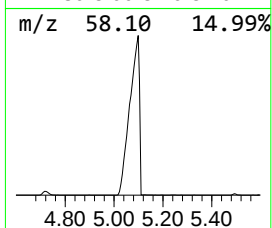
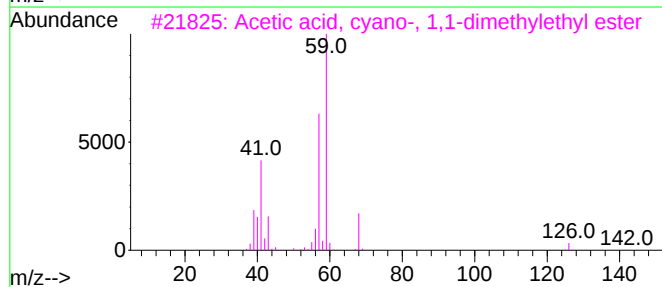
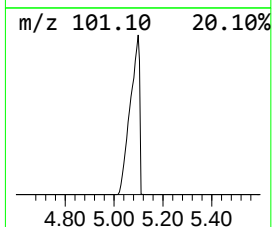
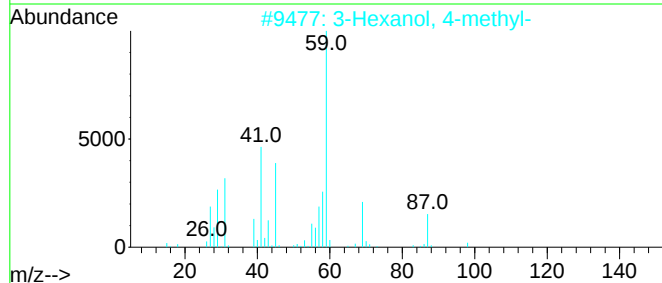
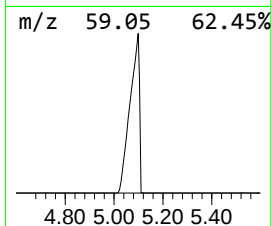
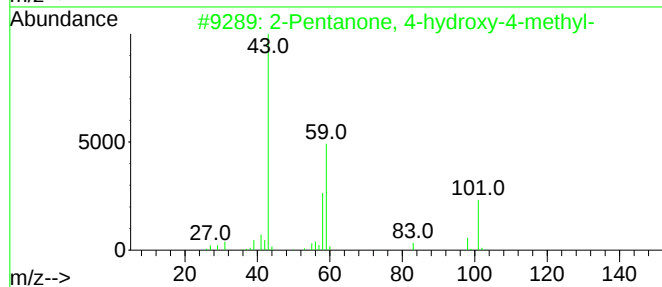
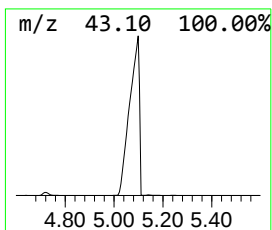
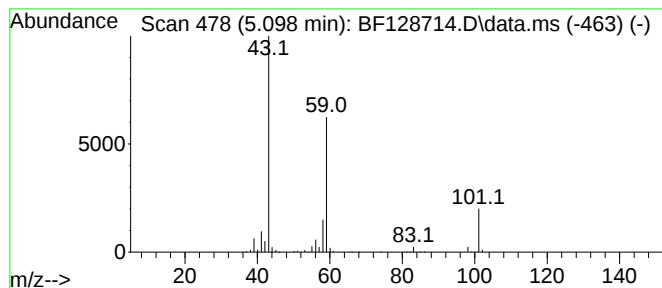
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	367.65 ng	9761290	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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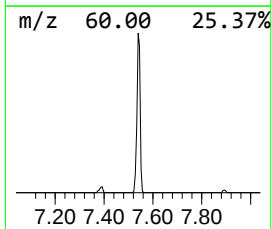
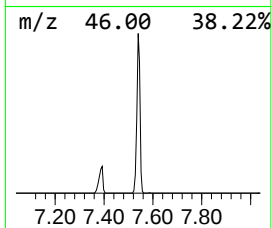
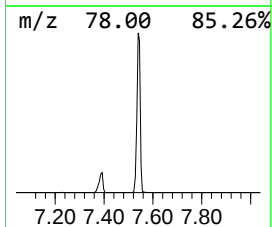
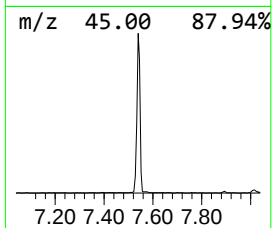
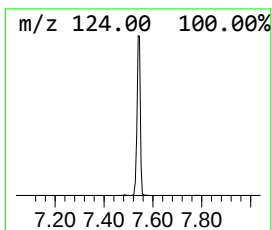
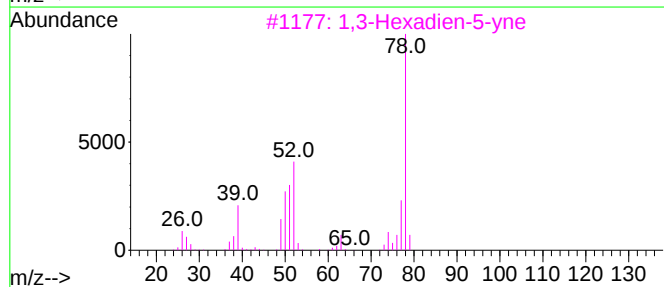
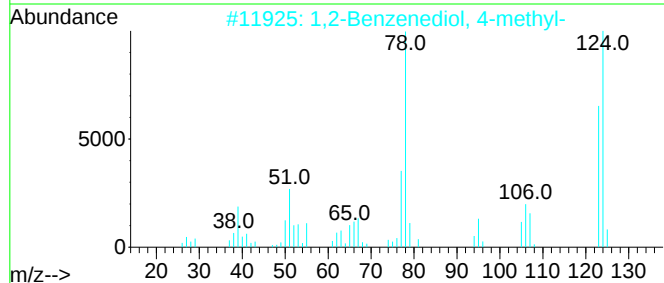
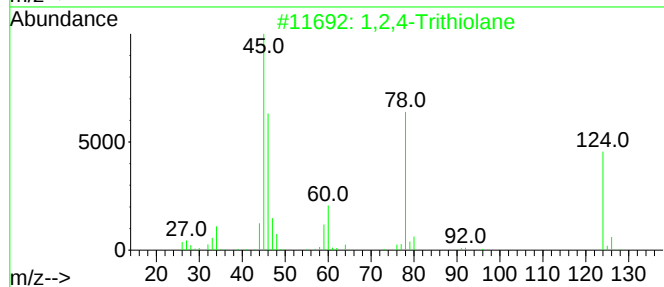
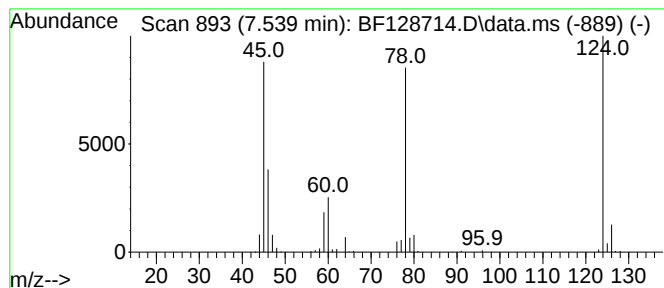
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,2,4-Trithiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.539	14.49 ng	492618	Naphthalene-d8	8.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	78
2			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	42
3			1,3-Hexadien-5-yne	78	C6H6	010420-90-3	25
4			Fumaronitrile	78	C4H2N2	000764-42-1	9
5			Benzene	78	C6H6	000071-43-2	9



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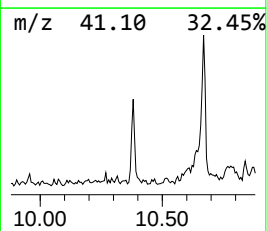
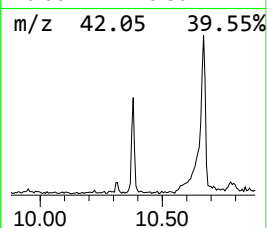
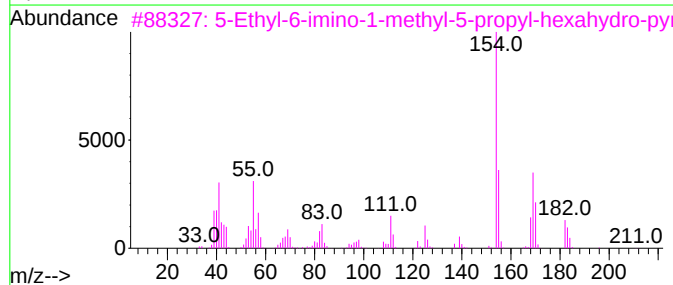
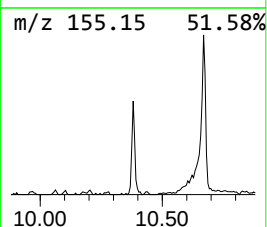
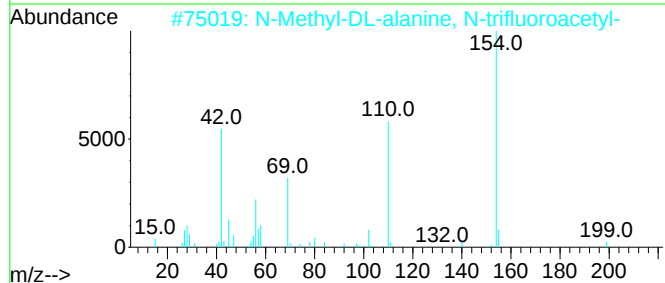
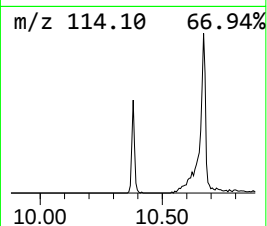
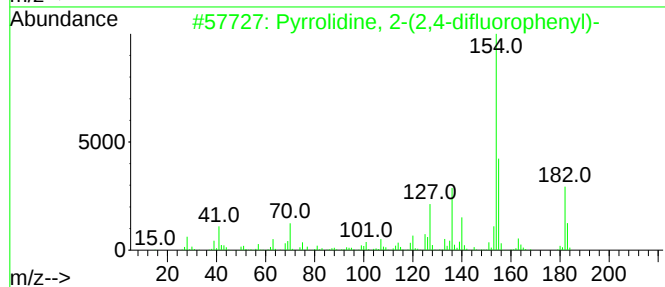
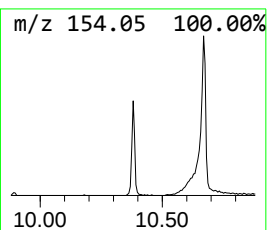
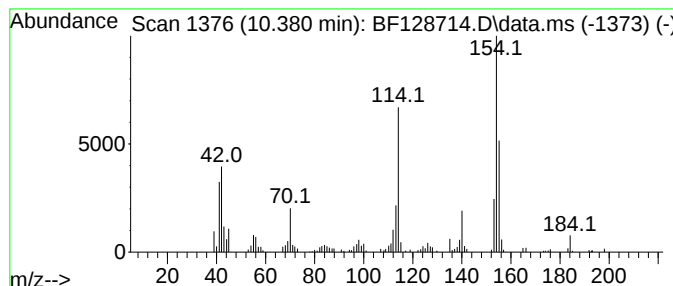
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.381 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.381	3.31 ng	128552	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrrolidine, 2-(2,4-difluorophen...	183	C10H11F2N	524674-05-3	43
2			N-Methyl-DL-alanine, N-trifluoro...	199	C6H8F3NO3	1000452-66-9	35
3			5-Ethyl-6-imino-1-methyl-5-propy...	211	C10H17N3O2	1000296-08-6	32
4			p-(Methylthio)benzyl alcohol	154	C8H10OS	003446-90-0	30
5			2,5-Dimethoxypyrimidin-4-amine	155	C6H9N3O2	006960-17-4	25



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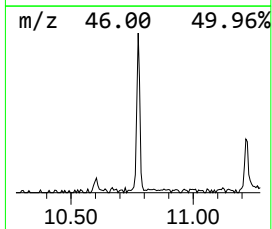
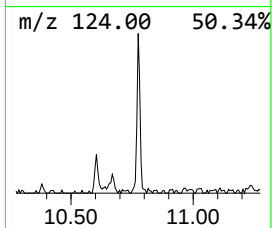
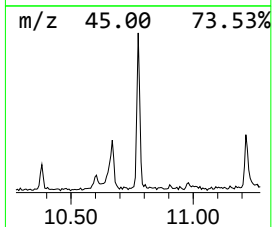
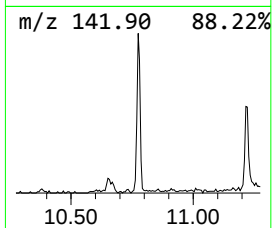
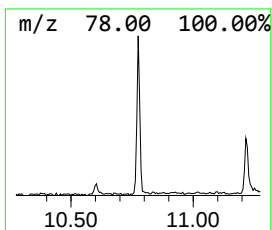
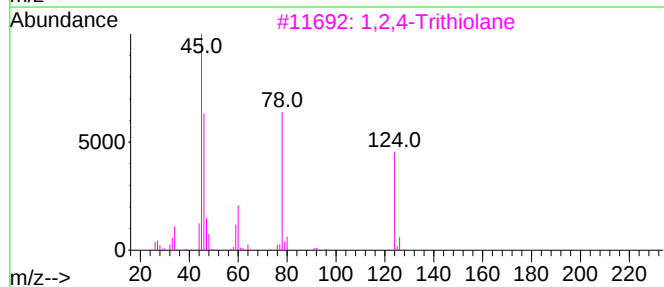
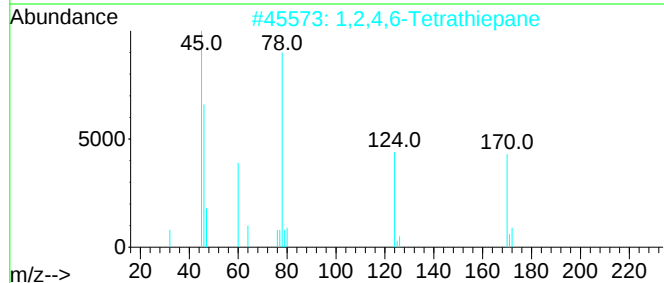
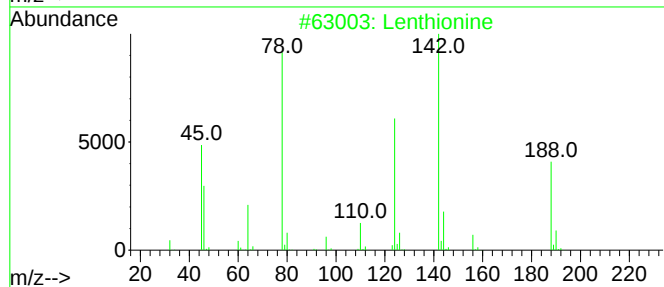
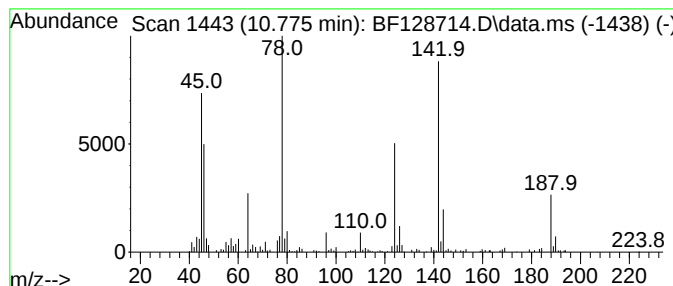
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Lenthionine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	3.96 ng	178530	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	95
2			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	37
4			Phenylphosphonous acid	142	C6H7O2P	001779-48-2	9
5			Benzene	78	C6H6	000071-43-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060722\
Data File : BF128714.D
Acq On : 07 Jun 2022 13:47
Operator : CG\JU
Sample : N3189-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220423-AMENDED-COMPOSITE-C

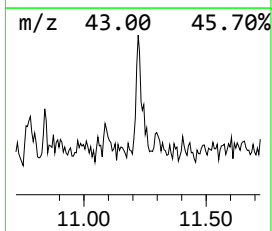
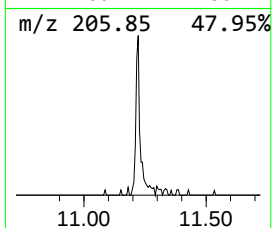
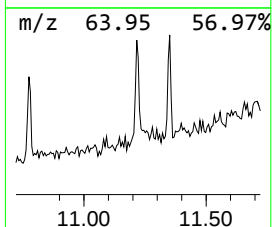
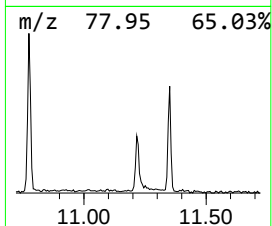
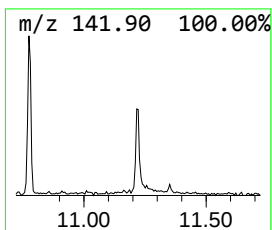
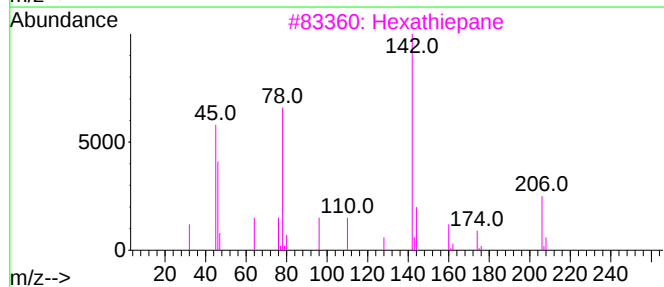
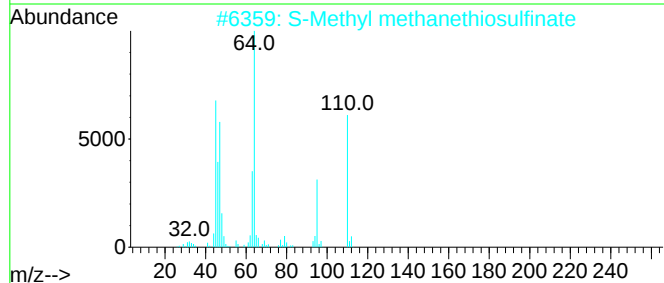
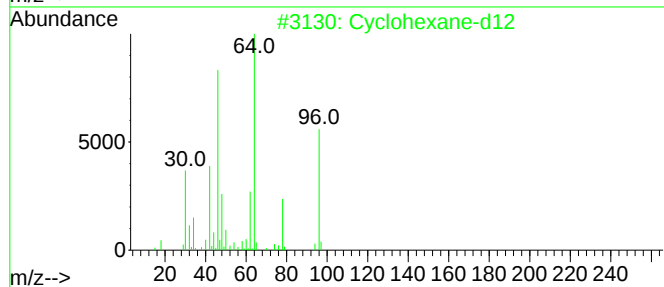
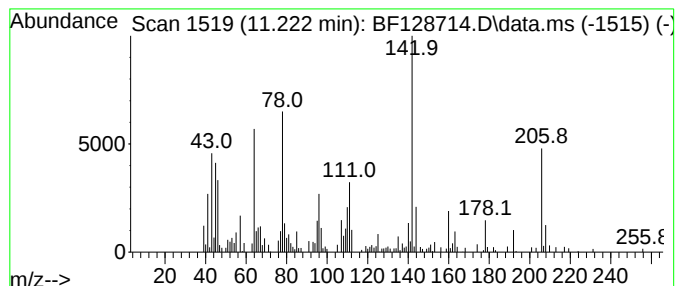
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown11.222 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.222	3.18 ng	143222	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane-d12	96	C6D12	001735-17-7	38
2			S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	17
3			Hexathiepane	206	CH2S6	017233-71-5	16
4			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	16
5			S-2-[2-Succinimidoethylamino]eth...	282	C8H14N2O5S2	031701-74-3	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060722\
Data File : BF128714.D
Acq On : 07 Jun 2022 13:47
Operator : CG\JU
Sample : N3189-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220423-AMENDED-COMPOSITE-C

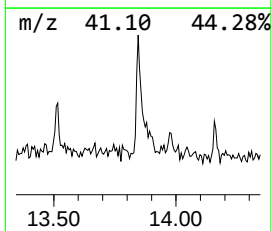
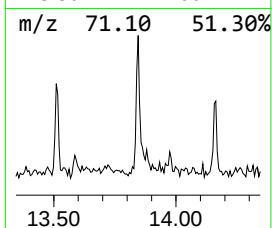
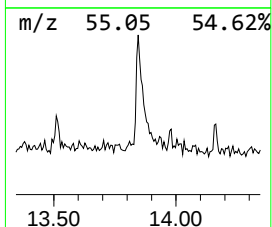
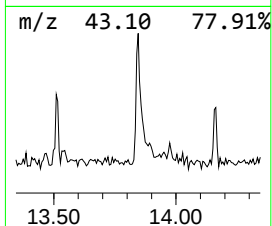
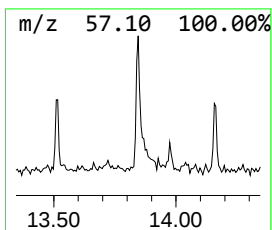
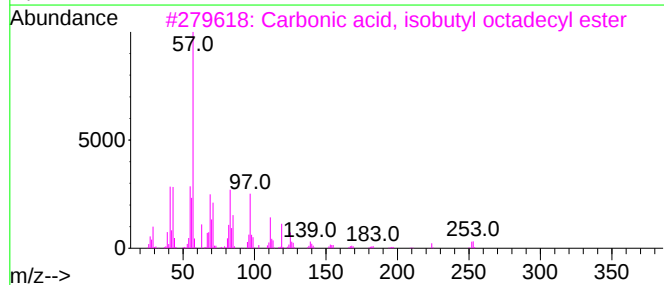
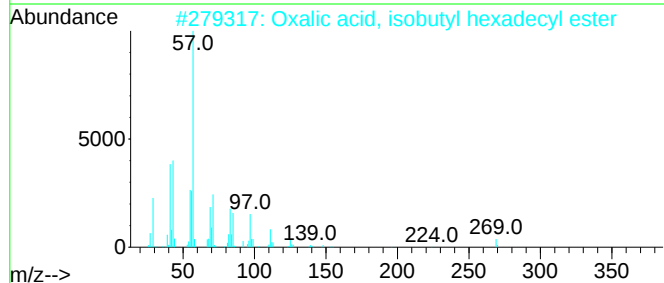
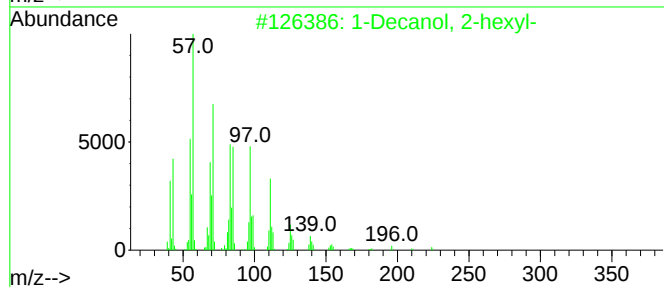
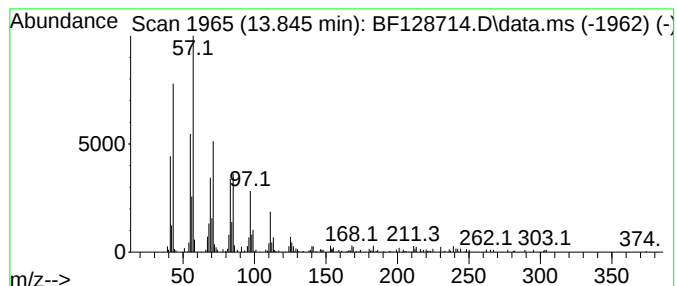
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.60 ng	190544	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	91
2	Oxalic acid, isobutyl hexadecyl ...			370	C22H42O4	1000309-38-1	76
3	Carbonic acid, isobutyl octadecyl...			370	C23H46O3	1000314-61-5	74
4	Oxalic acid, isobutyl octadecyl ...			398	C24H46O4	1000309-38-3	68
5	1-Dodecanol, 2-octyl-			298	C20H42O	005333-42-6	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060722\
Data File : BF128714.D
Acq On : 07 Jun 2022 13:47
Operator : CG\JU
Sample : N3189-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220423-AMENDED-COMPOSITE-C

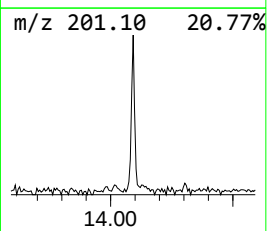
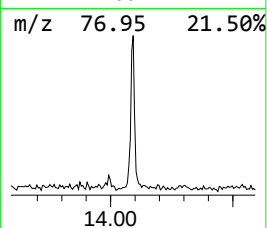
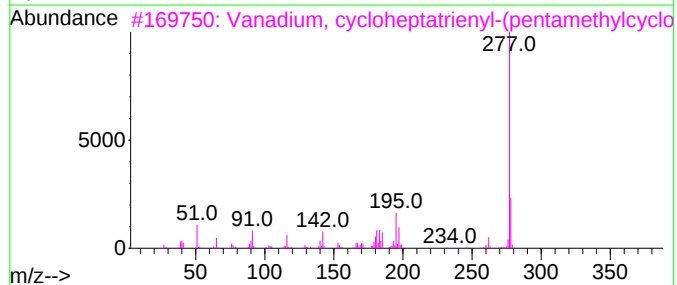
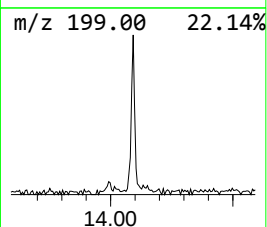
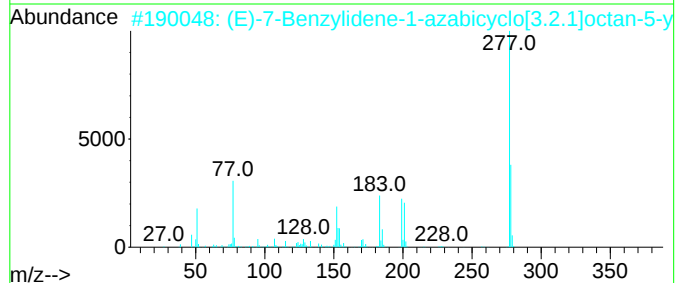
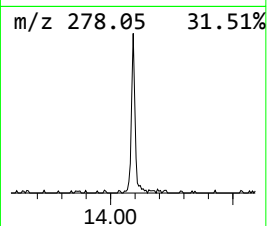
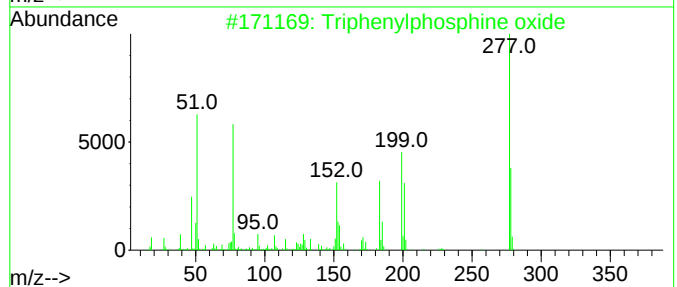
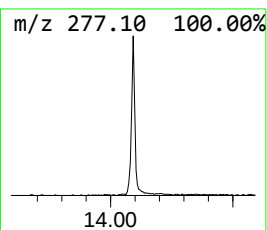
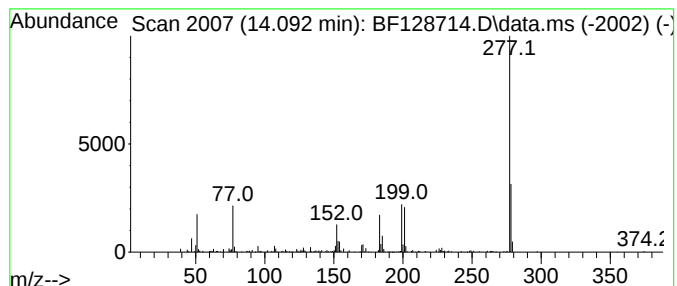
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	4.81 ng	163773	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	99
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	58
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060722\
Data File : BF128714.D
Acq On : 07 Jun 2022 13:47
Operator : CG\JU
Sample : N3189-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220423-AMENDED-COMPOSITE-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
Propylene Glycol	3.451	14.0	ng	370658	1	6.822	531010	20.0
2-Pentanone, 4-...	4.722	4.0	ng	104859	1	6.822	531010	20.0
2-Pentanone, 4-...	5.098	367.6	ng	9761290	1	6.822	531010	20.0
1,2,4-Trithiolane	7.539	14.5	ng	492618	2	8.104	680071	20.0
unknown10.381	10.381	3.3	ng	128552	3	9.863	777649	20.0
Lenthionine	10.775	4.0	ng	178530	4	11.351	900885	20.0
unknown11.222	11.222	3.2	ng	143222	4	11.351	900885	20.0
1-Decanol, 2-he...	13.845	5.6	ng	190544	5	13.998	680915	20.0
Triphenylphosph...	14.092	4.8	ng	163773	5	13.998	680915	20.0