

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
 Data File : BF138551.D
 Acq On : 12 Jul 2024 17:35
 Operator : CG\JU
 Sample : P3207-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHRT-24849

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	5	11	18	rBV	1460341	1793624	95.27%	12.976%
2	5.081	506	509	516	rVB	114875	124544	6.62%	0.901%
3	5.487	574	578	582	rBV	1780523	1619120	86.00%	11.713%
4	6.498	745	750	753	rBV	1903157	1679230	89.19%	12.148%
5	6.863	808	812	815	rBV	682834	516200	27.42%	3.734%
6	7.428	903	908	911	rBV	1247450	1126305	59.82%	8.148%
7	8.145	1026	1030	1033	rBV	818263	648325	34.44%	4.690%
8	8.451	1079	1082	1091	rBV	50113	55613	2.95%	0.402%
9	9.216	1207	1212	1216	rBV	2062888	1882742	100.00%	13.620%
10	9.604	1276	1278	1279	rBV	87182	67718	3.60%	0.490%
11	9.710	1294	1296	1300	rBV4	142168	158554	8.42%	1.147%
12	9.769	1303	1306	1308	rBV4	107969	143041	7.60%	1.035%
13	9.810	1310	1313	1315	rVB2	173448	210428	11.18%	1.522%
14	9.898	1325	1328	1332	rVB	849640	727822	38.66%	5.265%
15	10.310	1395	1398	1400	rBV	524461	488396	25.94%	3.533%
16	12.969	1847	1850	1859	rVB	1475460	1511216	80.27%	10.933%
17	14.022	2026	2029	2032	rVB	501579	465440	24.72%	3.367%
18	14.504	2109	2111	2120	rVB2	131667	151490	8.05%	1.096%
19	15.486	2273	2278	2287	rVB	324796	453147	24.07%	3.278%

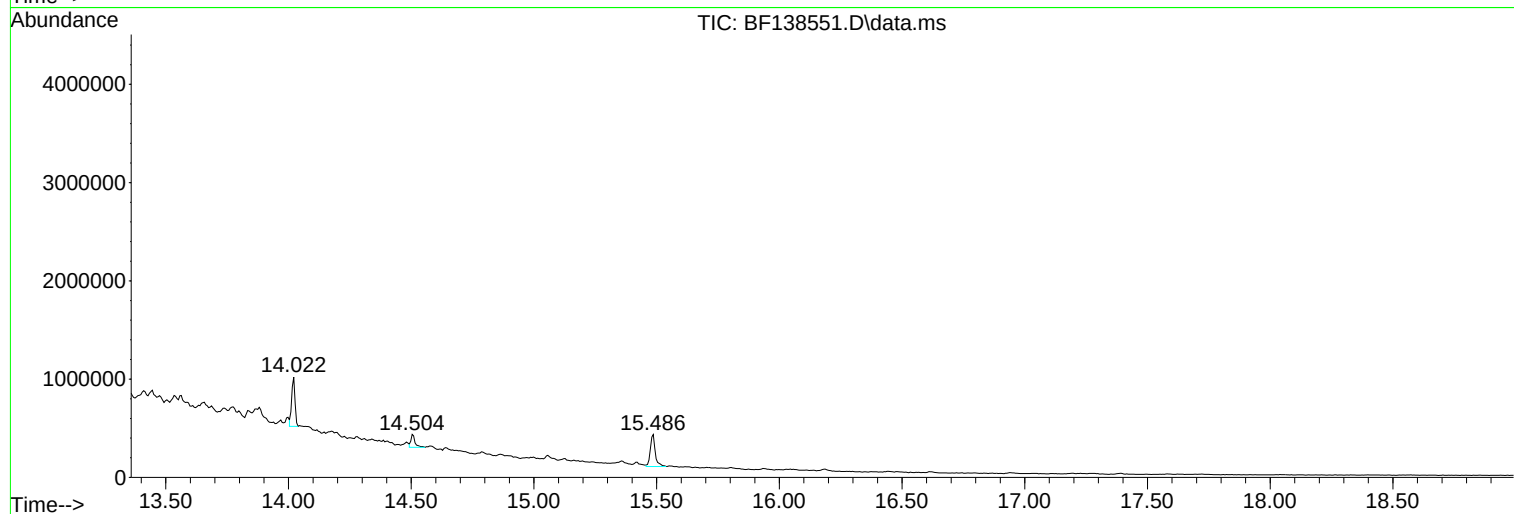
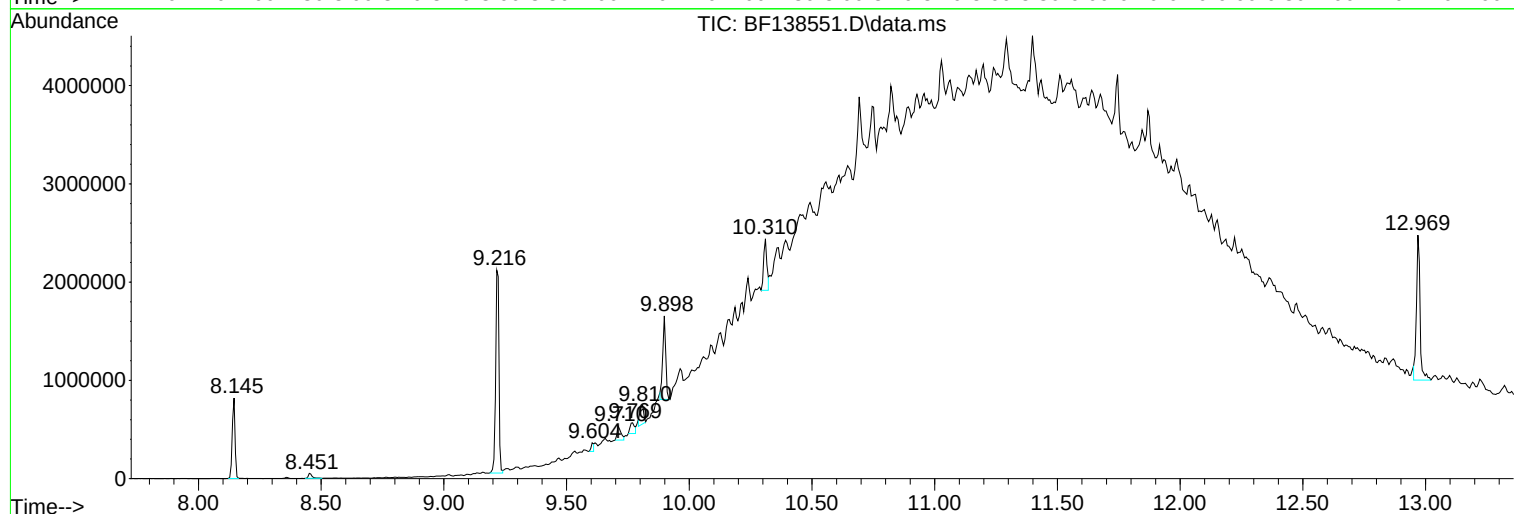
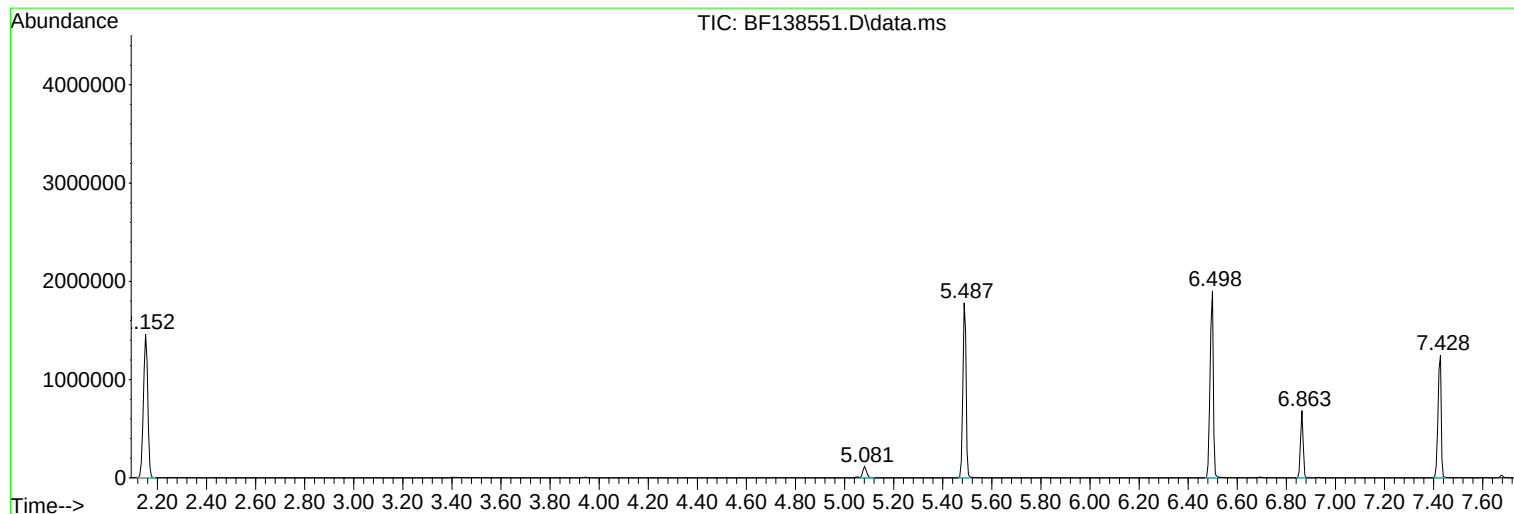
Sum of corrected areas: 13822955

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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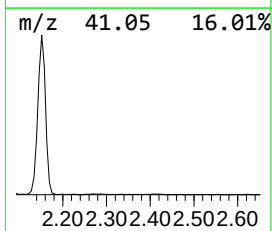
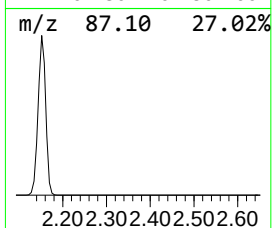
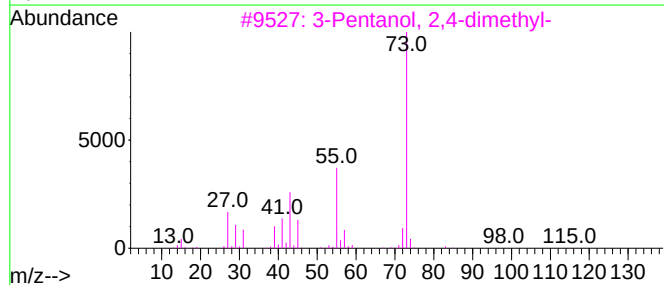
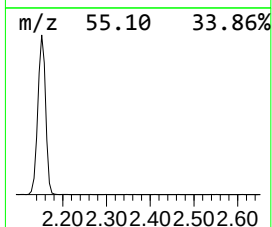
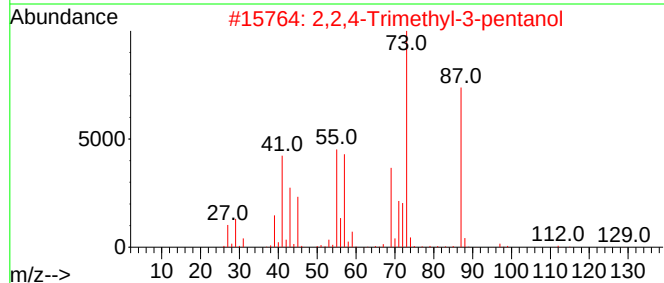
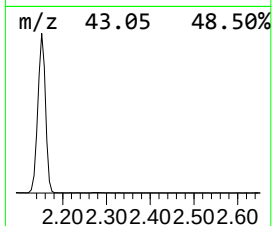
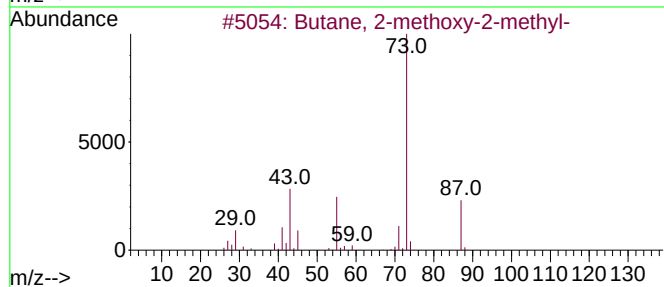
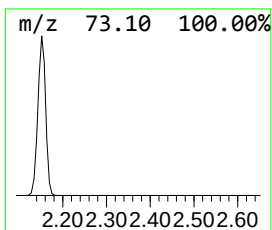
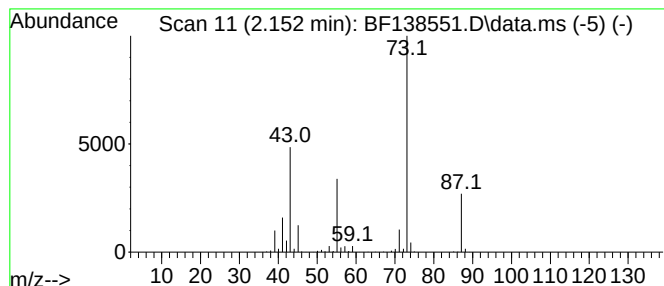
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.152	69.49 ng	1793620	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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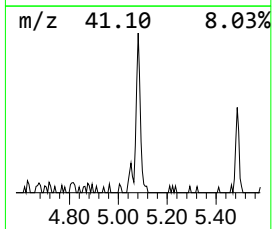
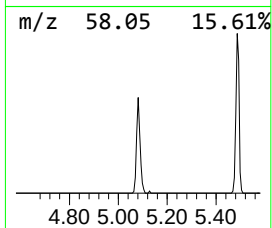
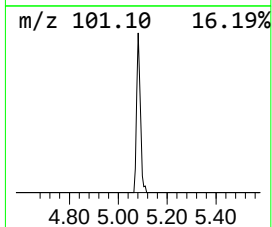
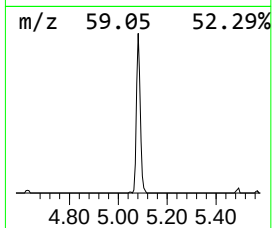
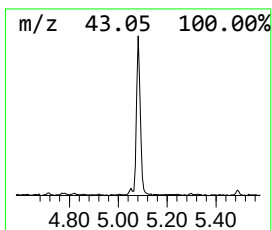
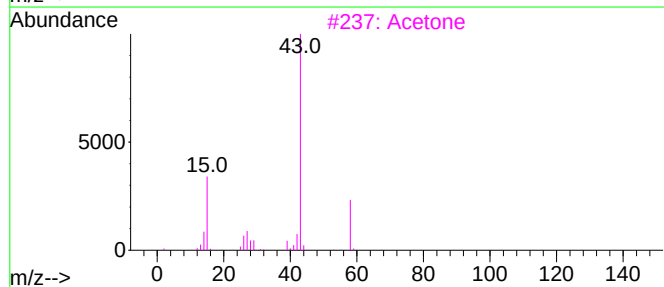
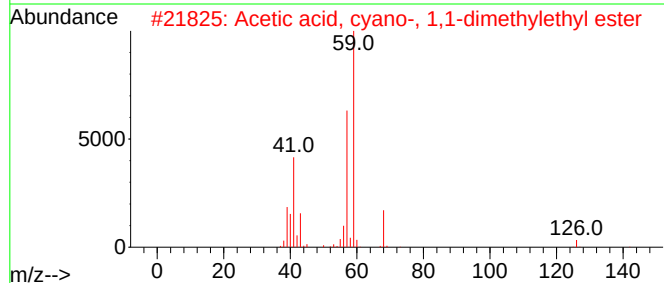
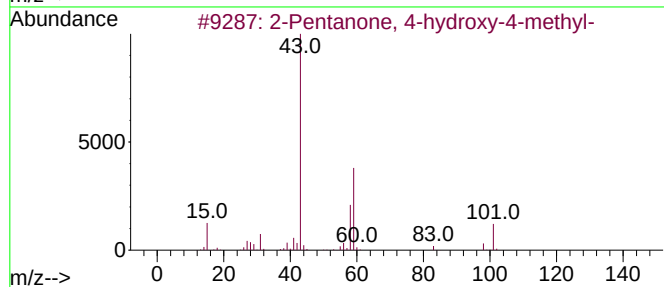
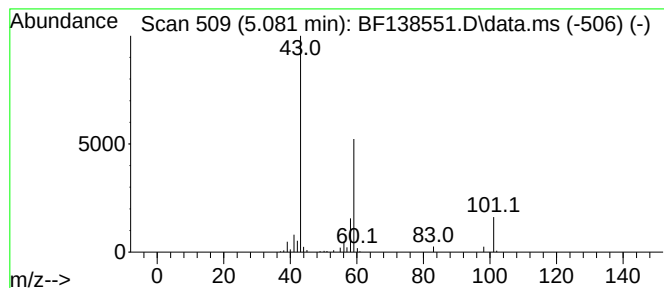
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.081	4.83 ng	124544	1,4-Dichlorobenzene-d4			6.863
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, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
3	Acetone		58	C3H6O	000067-64-1	12
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9



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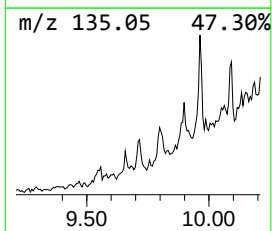
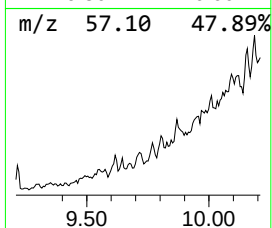
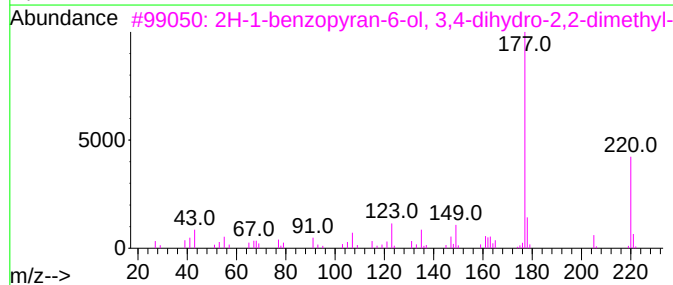
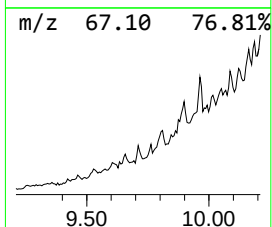
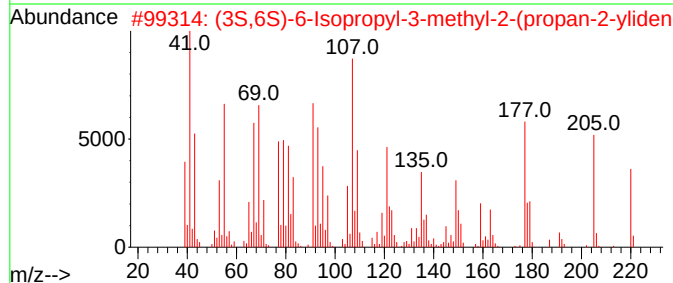
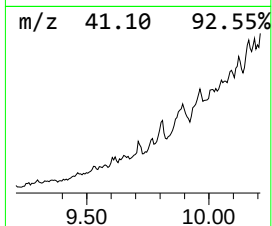
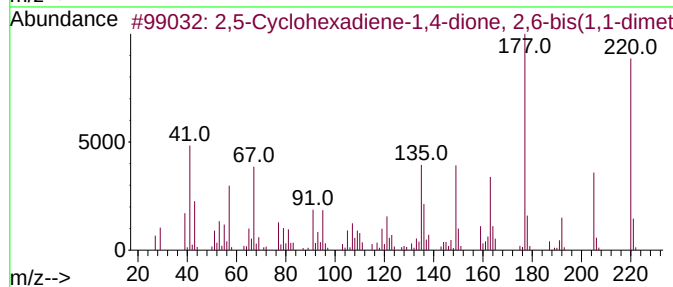
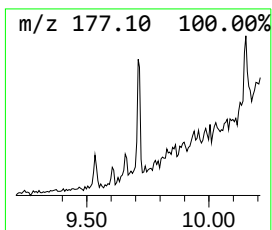
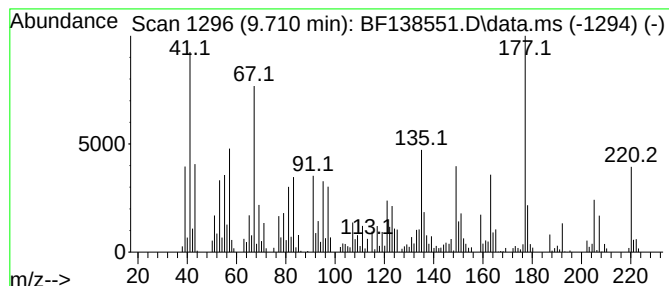
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Peak Number 3 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	4.36 ng	158554	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	93
2			(3S,6S)-6-Isopropyl-3-methyl-2-(...	220	C15H24O	021698-46-4	43
3			2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	41
4			1H-indene-4,7-diol, 2,3-dihydro-...	220	C14H20O2	1000396-25-5	38
5			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	30



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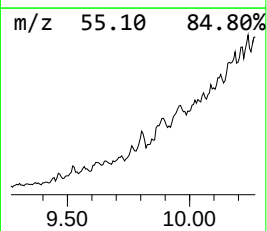
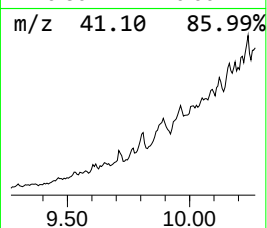
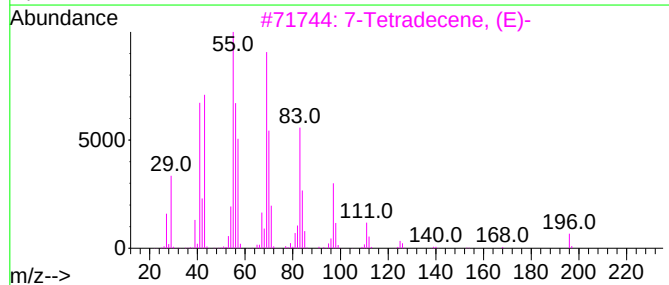
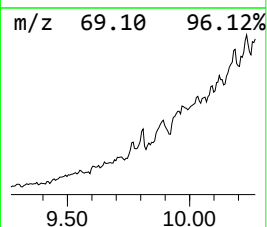
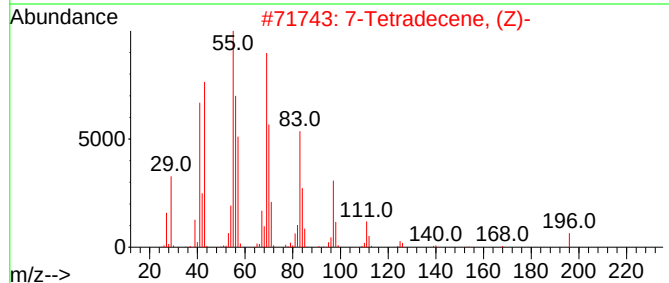
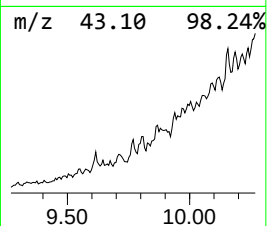
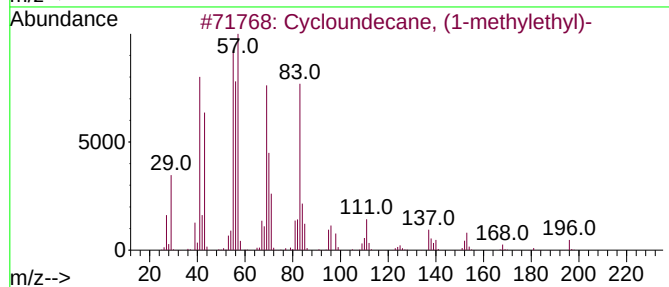
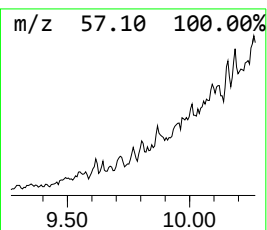
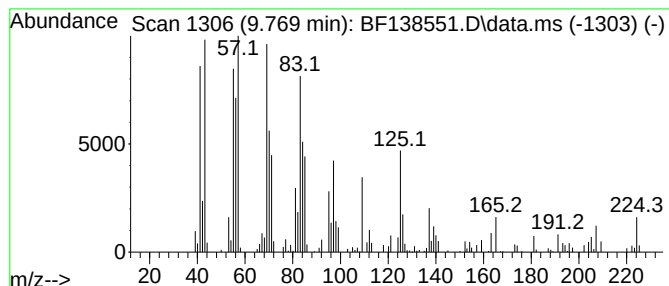
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Peak Number 4 Cycloundecane, (1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	3.93 ng	143041	Acenaphthene-d10	9.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloundecane, (1-methylethyl)-	196	C14H28	062338-56-1	62
2		7-Tetradecene, (Z)-	196	C14H28	041446-60-0	58
3		7-Tetradecene, (E)-	196	C14H28	041446-63-3	55
4		7-Tetradecene	196	C14H28	010374-74-0	49
5		3-Hexadecene, (Z)-	224	C16H32	034303-81-6	49



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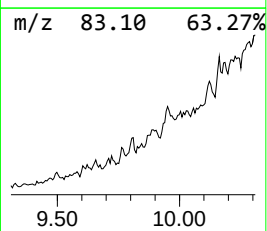
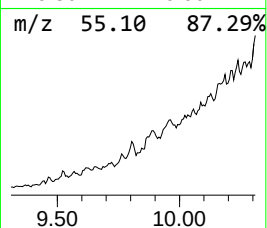
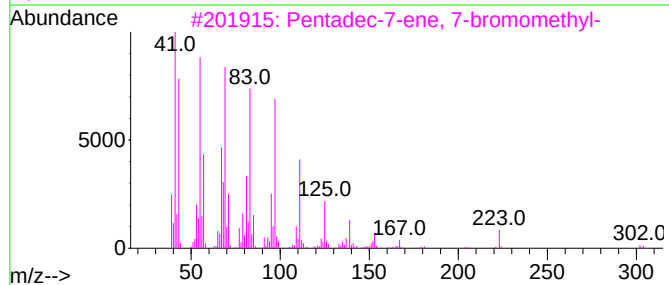
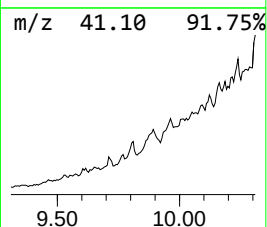
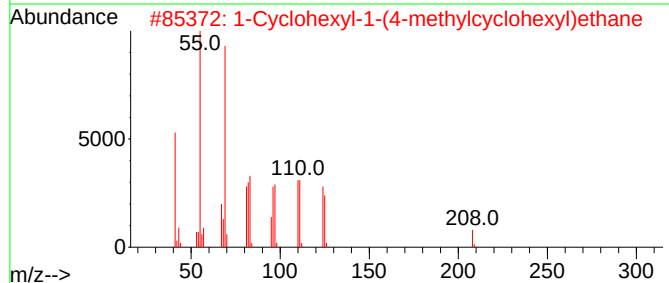
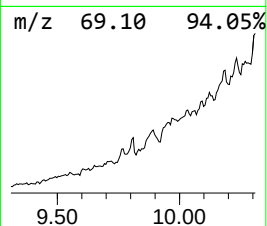
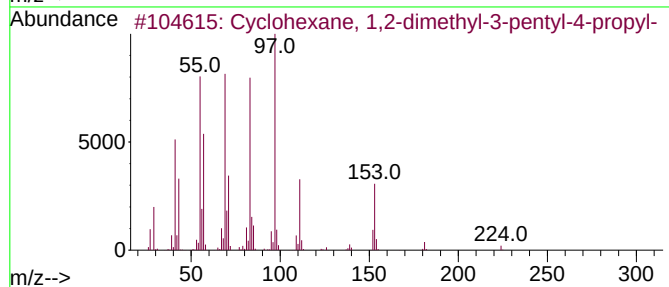
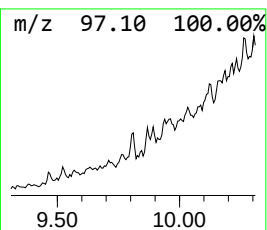
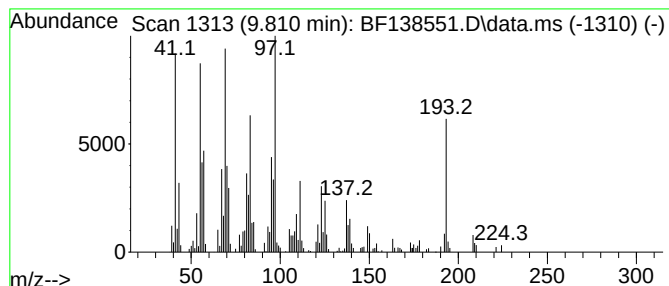
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Peak Number 5 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.810	5.78 ng	210428	Acenaphthene-d10	9.898	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	70
2	1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5	50
3	Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	49
4	4-Hexen-3-one, 4,5-dimethyl-	126	C8H14O	017325-90-5	30
5	2-Butenoic acid, 2-methyl-, 3-me...	168	C10H16O2	083783-86-2	30



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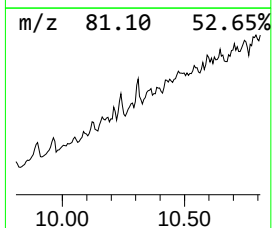
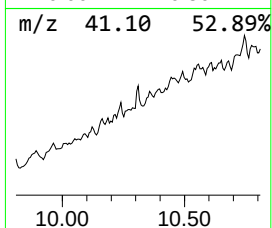
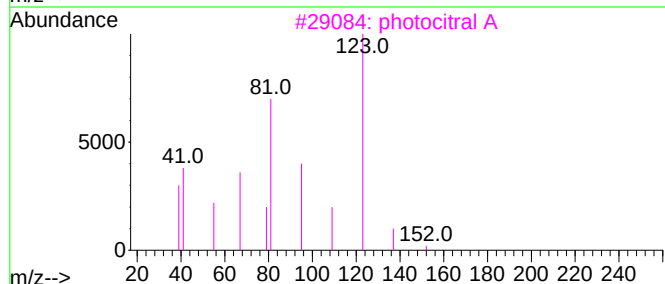
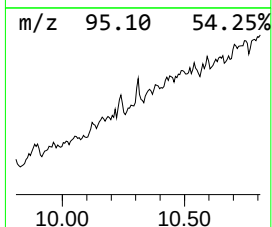
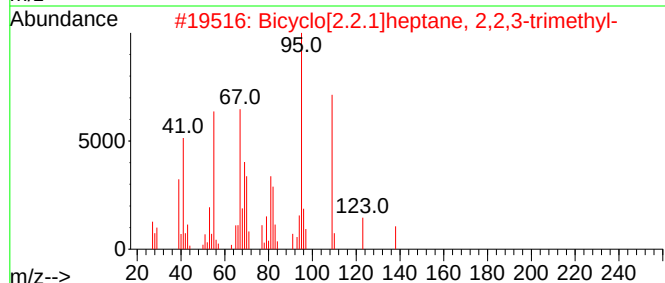
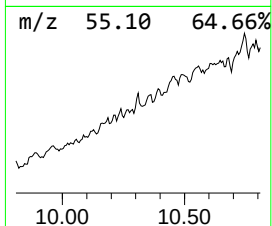
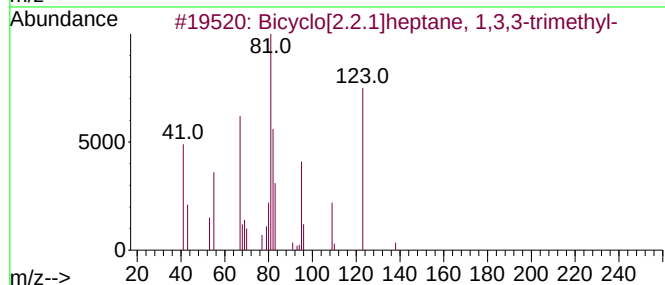
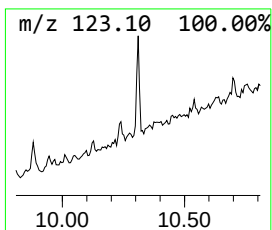
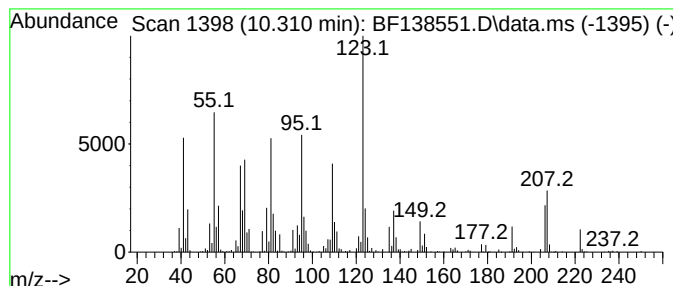
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.310 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.310	13.42 ng	488396	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	46
2			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	42
3			photocitral A	152	C10H16O	055253-28-6	38
4			1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	38
5			Pyridine-3-carboxylic acid, 1-[(...	290	C15H18N2O4	1010310-27-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138551.D
Acq On : 12 Jul 2024 17:35
Operator : CG\JU
Sample : P3207-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24849

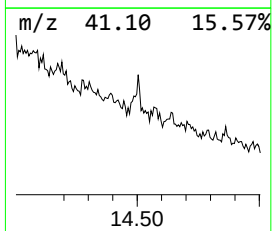
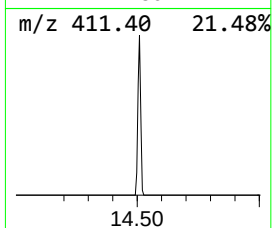
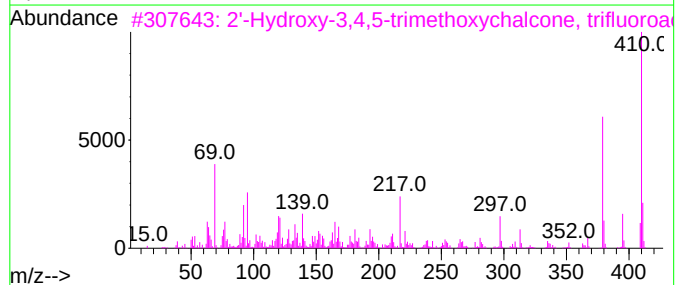
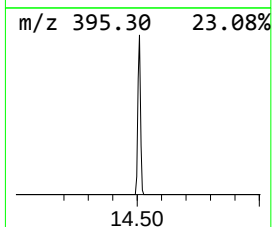
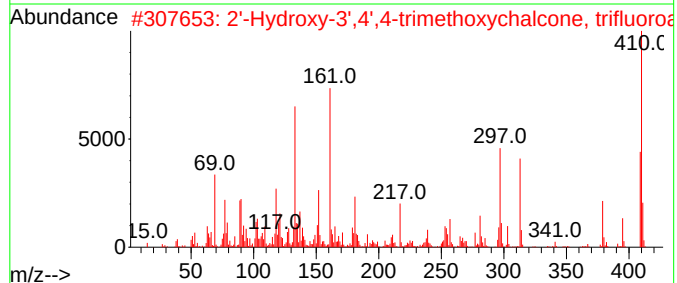
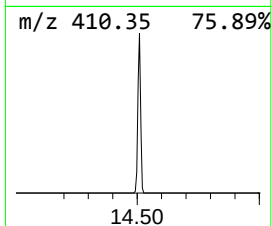
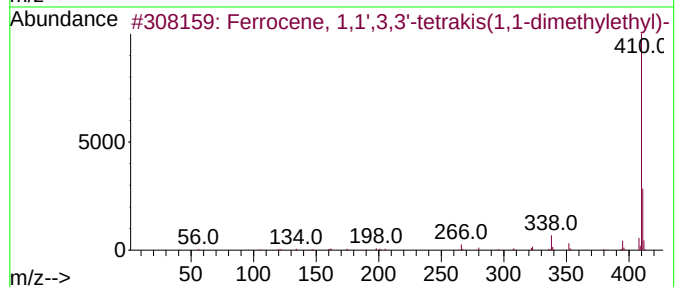
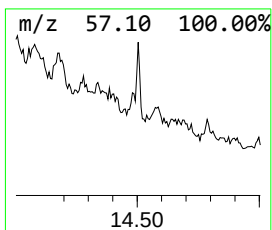
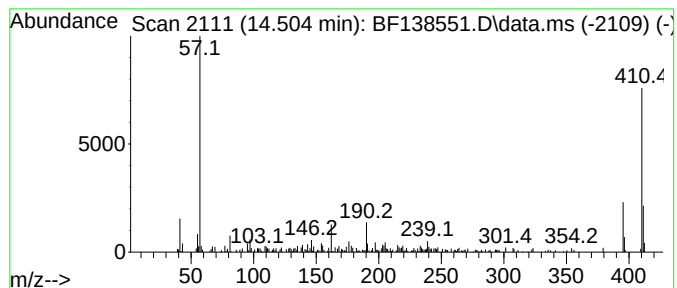
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.504 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	6.51 ng	151490	Chrysene-d12	14.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	49
2			2'-Hydroxy-3',4',4-trimethoxycha...	410	C20H17F3O6	1000449-45-6	40
3			2'-Hydroxy-3,4,5-trimethoxychalc...	410	C20H17F3O6	1000449-43-8	40
4			6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	38
5			3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138551.D
Acq On : 12 Jul 2024 17:35
Operator : CG\JU
Sample : P3207-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24849

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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...	2.152	69.5	ng	1793620	1	6.863	516200	20.0
2-Pentanone, 4-...	5.081	4.8	ng	124544	1	6.863	516200	20.0
2,5-Cyclohexadi...	9.710	4.4	ng	158554	3	9.898	727822	20.0
Cycloundecane, ...	9.769	3.9	ng	143041	3	9.898	727822	20.0
Cyclohexane, 1,...	9.810	5.8	ng	210428	3	9.898	727822	20.0
unknown10.310	10.310	13.4	ng	488396	3	9.898	727822	20.0
unknown14.504	14.504	6.5	ng	151490	5	14.022	465440	20.0