

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
 Data File : BF138556.D
 Acq On : 12 Jul 2024 20:08
 Operator : CG\JU
 Sample : P3207-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-2929

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: BF138556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	503	506	511	rVB	144418	154573	5.03%	0.319%
2	5.487	574	578	591	rVB	1893630	1942395	63.16%	4.007%
3	6.498	744	750	754	rBV	2174787	1948700	63.37%	4.020%
4	6.863	809	812	817	rVB	753033	594366	19.33%	1.226%
5	7.428	904	908	911	rBV	1345306	1170614	38.07%	2.415%
6	8.010	1004	1007	1012	rBV	164709	152839	4.97%	0.315%
7	8.075	1014	1018	1021	rBV	3991819	3075271	100.00%	6.344%
8	8.145	1027	1030	1033	rVB	747555	552527	17.97%	1.140%
9	8.222	1040	1043	1047	rVB	232381	185417	6.03%	0.382%
10	8.345	1061	1064	1066	rBV	166817	136036	4.42%	0.281%
11	8.892	1154	1157	1159	rBV	266860	219028	7.12%	0.452%
12	9.128	1193	1197	1201	rBV4	121555	230465	7.49%	0.475%
13	9.222	1209	1213	1216	rBV	1588308	1427695	46.43%	2.945%
14	9.292	1222	1225	1229	rBV2	304588	396122	12.88%	0.817%
15	9.375	1236	1239	1242	rBV3	162629	179029	5.82%	0.369%
16	9.410	1242	1245	1248	rBV2	306592	329129	10.70%	0.679%
17	9.439	1248	1250	1252	rBV3	115628	134473	4.37%	0.277%
18	9.469	1252	1255	1258	rBV2	458426	545293	17.73%	1.125%
19	9.604	1276	1278	1283	rBV3	1235369	1798909	58.50%	3.711%
20	9.769	1302	1306	1308	rBV2	1219739	1268056	41.23%	2.616%
21	9.792	1308	1310	1311	rVV2	771161	597781	19.44%	1.233%
22	9.810	1311	1313	1316	rVB	1737970	1484265	48.26%	3.062%
23	9.863	1317	1322	1323	rBV3	625653	950771	30.92%	1.961%
24	9.880	1323	1325	1327	rVV	677234	749048	24.36%	1.545%
25	9.904	1327	1329	1332	rVB4	1060828	1006323	32.72%	2.076%
26	9.945	1332	1336	1338	rBV3	652569	945074	30.73%	1.950%
27	10.128	1365	1367	1369	rBV2	507962	466352	15.16%	0.962%
28	10.239	1381	1386	1390	rBV4	1421285	2533349	82.38%	5.226%
29	10.316	1396	1399	1401	rBV2	2584732	2270337	73.83%	4.684%
30	10.569	1439	1442	1446	rBV4	1140059	1826193	59.38%	3.767%
31	10.651	1453	1456	1458	rVB	1450998	1217640	39.59%	2.512%
32	10.775	1474	1477	1480	rBV	2436283	2374037	77.20%	4.897%
33	10.933	1501	1504	1508	rVB	1884157	1832863	59.60%	3.781%
34	11.145	1538	1540	1543	rBV2	1300207	1539913	50.07%	3.177%
35	15.039	2199	2202	2207	rVB	1761481	1802629	58.62%	3.719%
36	15.374	2256	2259	2264	rVB	935163	1183799	38.49%	2.442%

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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

37	15.780	2324	2328	2338	rVB	867037	1764347	57.37%	3.640%
38	15.998	2360	2365	2370	rVB	1581367	2497141	81.20%	5.151%
39	16.498	2445	2450	2460	rVB	1218302	2226074	72.39%	4.592%
40	18.080	2714	2719	2728	rVB	1118592	2766200	89.95%	5.706%

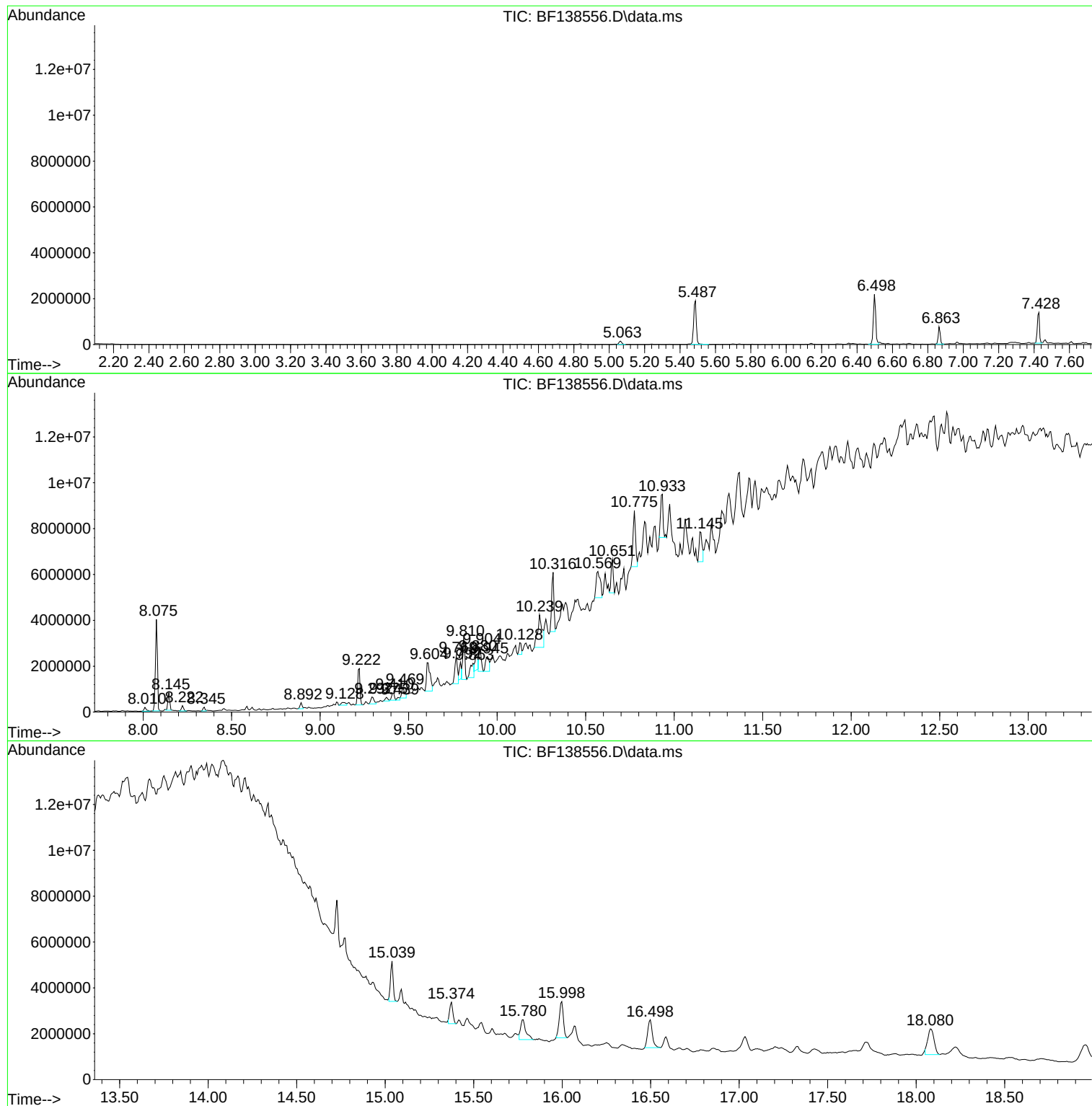
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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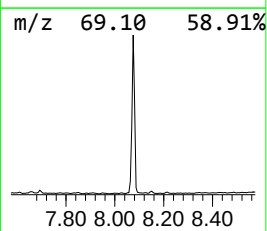
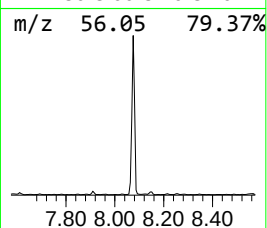
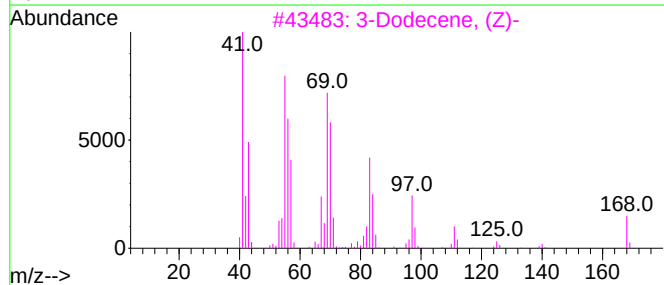
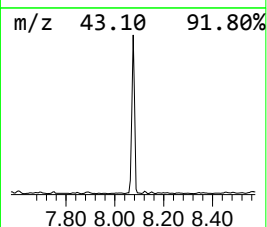
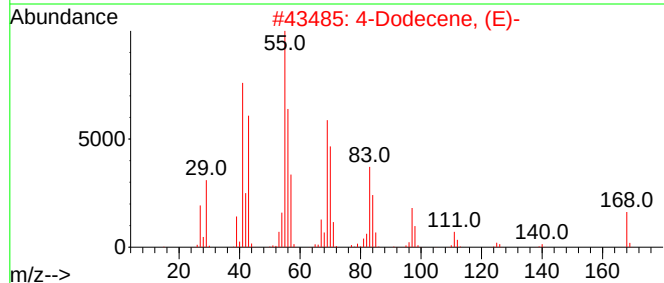
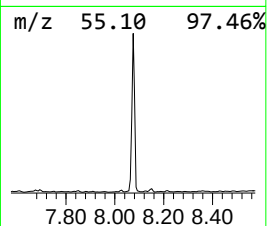
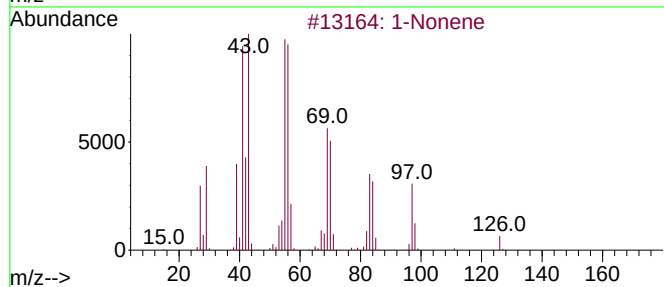
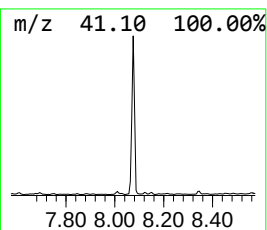
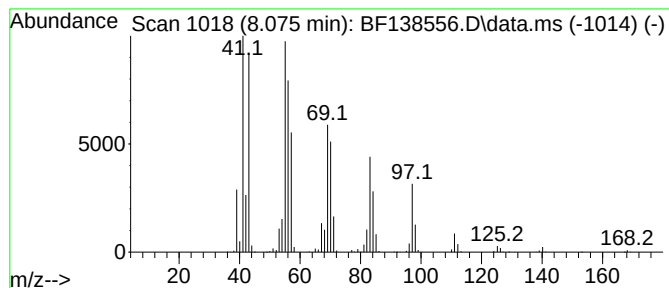
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Nonene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	111.32 ng	3075270	Naphthalene-d8	8.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonene			126	C9H18	000124-11-8	93
2	4-Dodecene, (E)-			168	C12H24	007206-15-7	91
3	3-Dodecene, (Z)-			168	C12H24	007239-23-8	91
4	2-Dodecene, (E)-			168	C12H24	007206-13-5	91
5	E-11,13-Tetradecadien-1-ol			210	C14H26O	1000131-00-3	91



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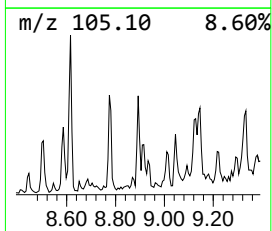
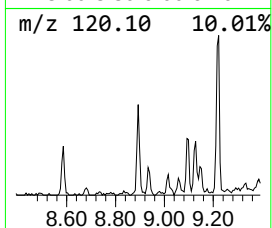
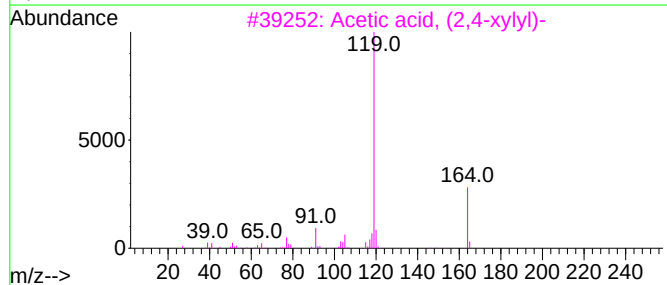
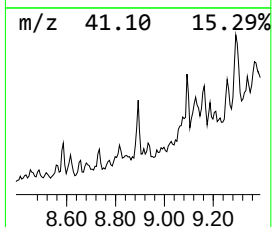
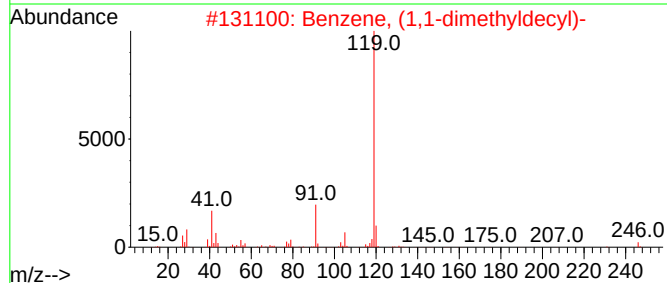
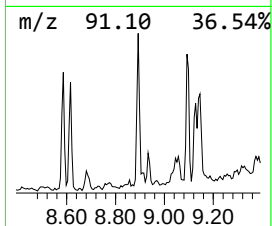
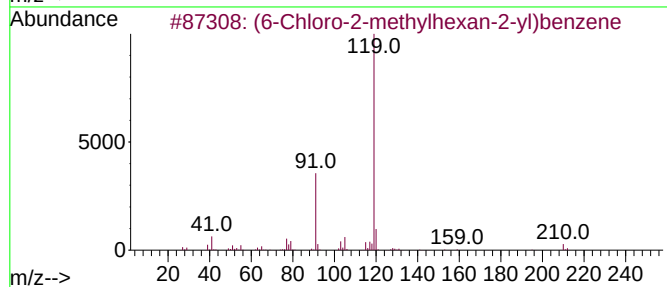
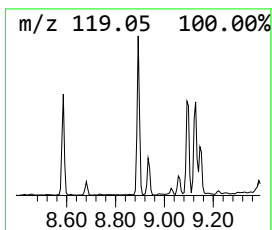
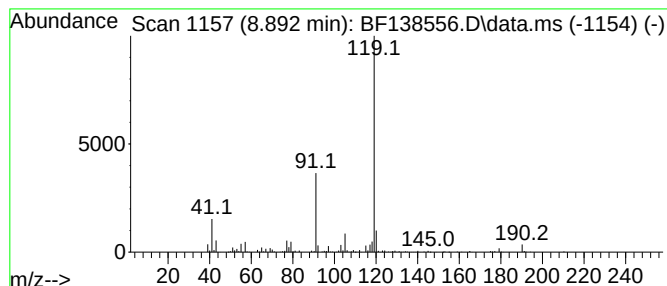
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (6-Chloro-2-methylhexan-2-yl... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.892	7.93 ng	219028	Naphthalene-d8	8.145

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	90
2		Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	78
3		Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	78
4		2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	78
5		Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	78



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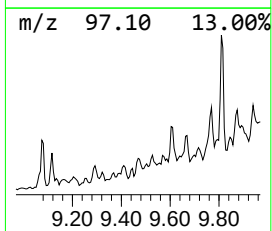
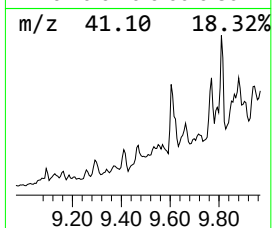
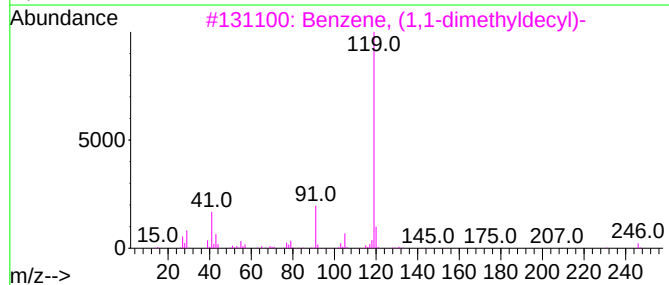
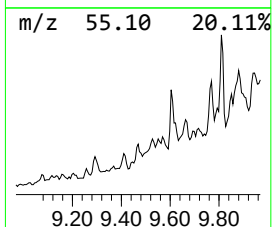
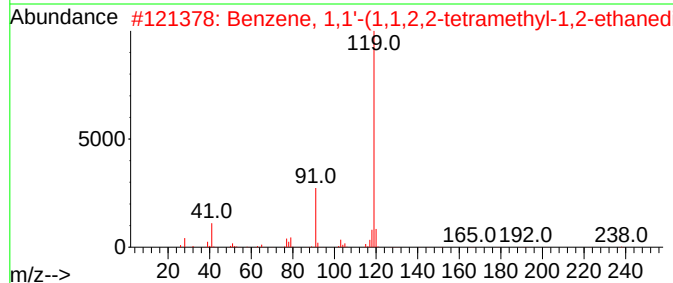
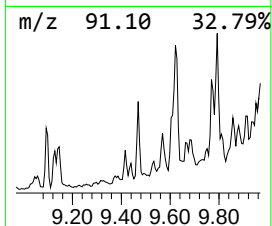
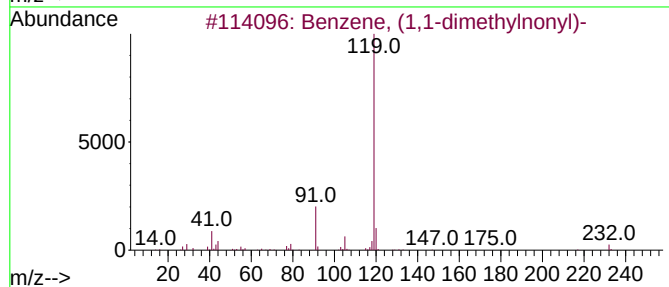
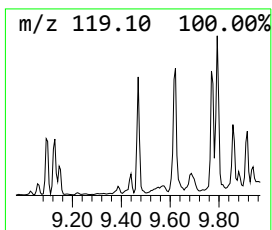
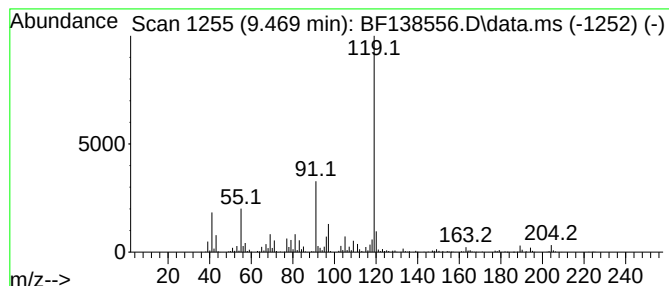
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, (1,1-dimethylnonyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.469	10.84 ng	545293	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	59
2			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	59
3			Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	59
4			2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	59
5			Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	59



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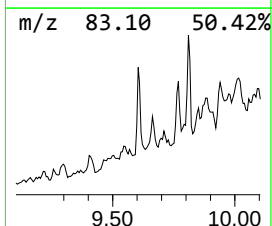
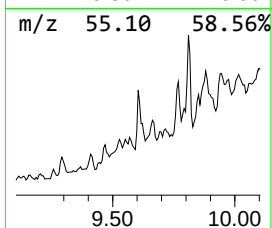
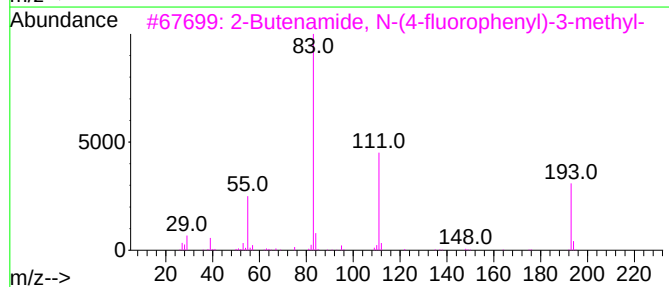
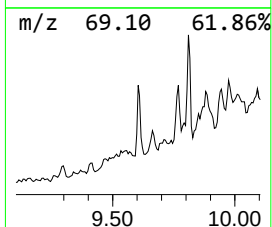
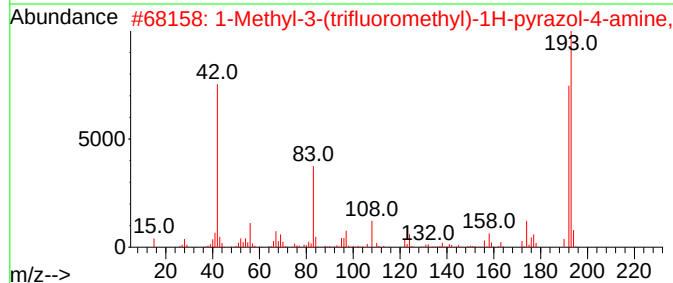
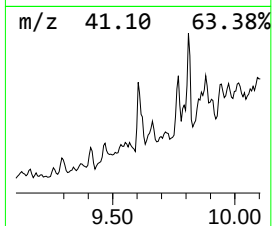
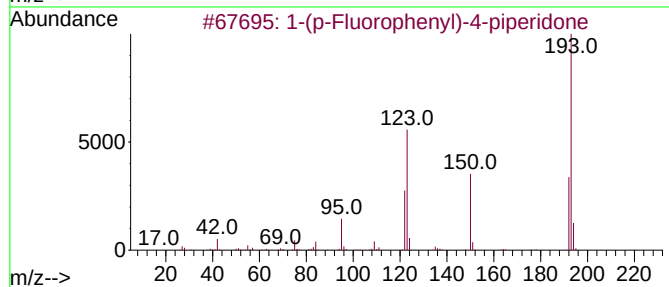
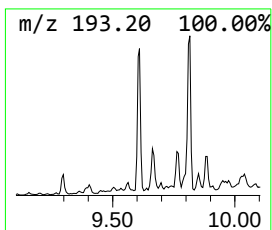
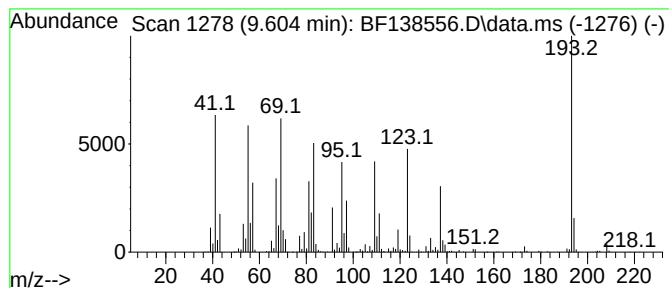
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown9.604 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	35.75 ng	1798910	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
2	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	35		
3	2-Butenamide, N-(4-fluorophenyl)...	193	C11H12FNO	1000307-26-7	30		
4	2-Anthracenamine	193	C14H11N	000613-13-8	25		
5	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	22		



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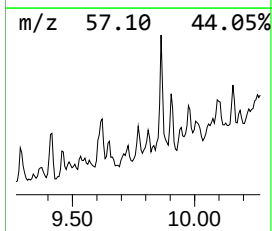
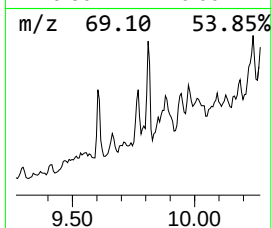
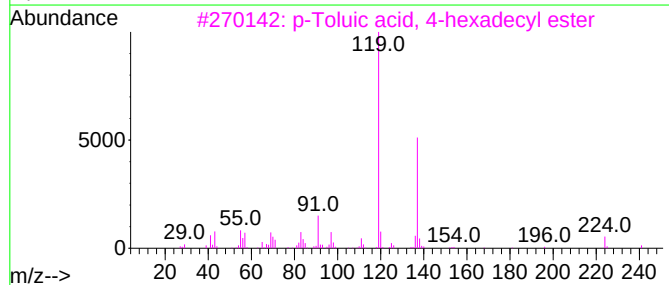
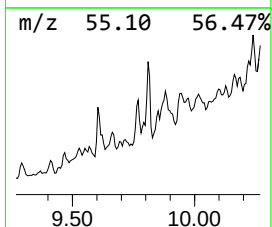
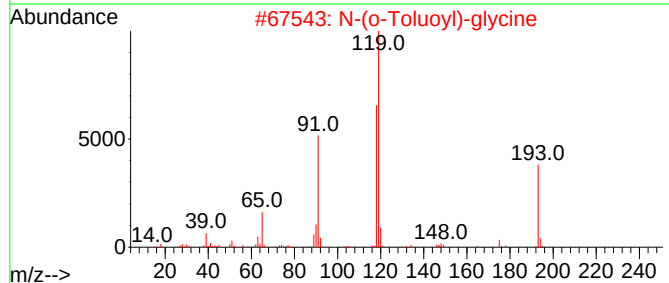
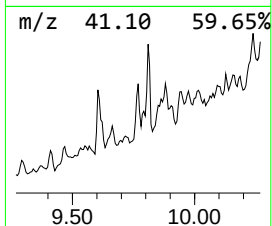
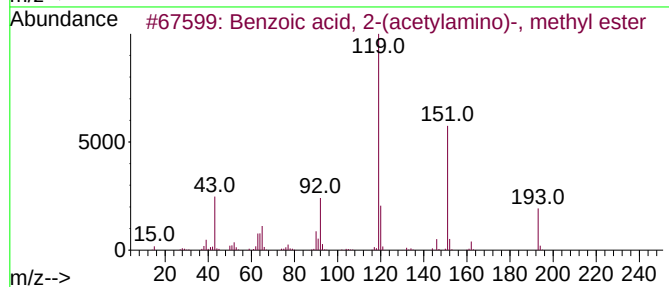
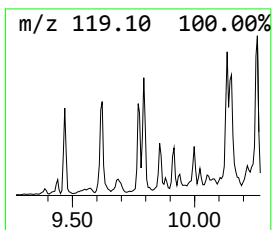
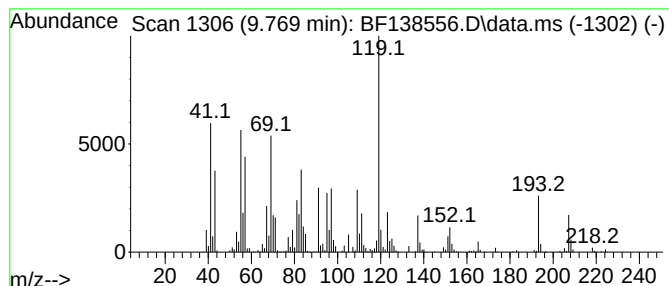
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.769 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	25.20 ng	1268060	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(acetylamo-	193	C10H11NO3	002719-08-6	35
2			N-(o-Toluoyl)-glycine	193	C10H11NO3	042013-20-7	35
3			p-Toluic acid, 4-hexadecyl ester	360	C24H40O2	1000292-22-1	27
4			Glycine, N-(4-methylbenzoyl)-, m...	207	C11H13NO3	001208-23-7	27
5			m-Toluic acid, 5-tetradecyl ester	332	C22H36O2	1000299-78-5	27



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Operator : CG\JU
Sample : P3207-07
Misc :
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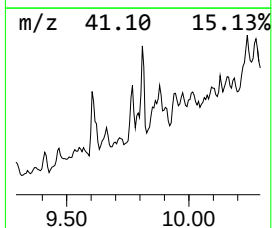
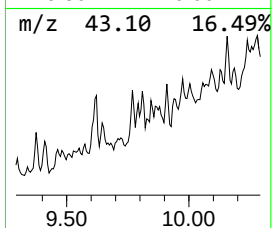
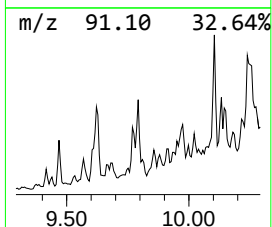
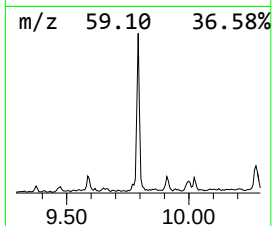
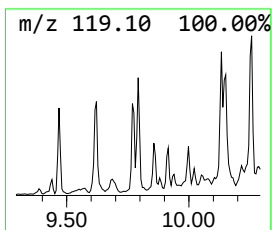
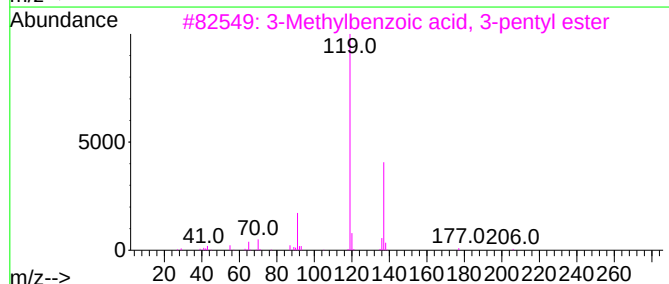
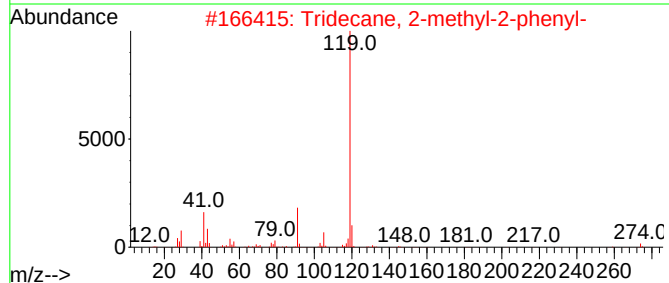
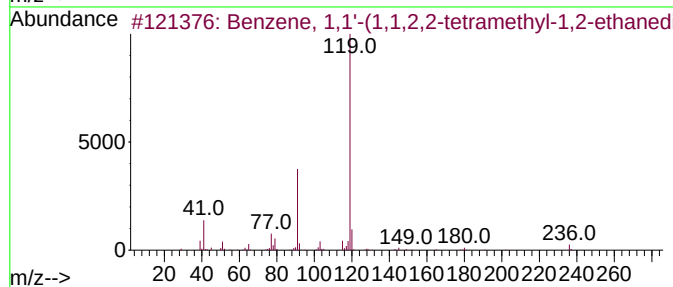
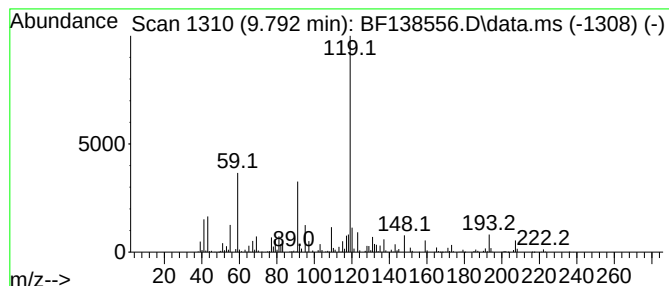
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1,1'-(1,1,2,2-tetr... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.792	11.88 ng	597781	Acenaphthene-d10	9.898	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	60
2	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	47
3	3-Methylbenzoic acid, 3-pentyl e...	206	C13H18O2	1000325-71-1	47
4	3,5-Dimethylbenzylnonylamine	261	C18H31N	1010491-61-1	47
5	Benzene, isocyanato-	119	C7H5NO	000103-71-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
Operator : CG\JU
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ClientSampleId :
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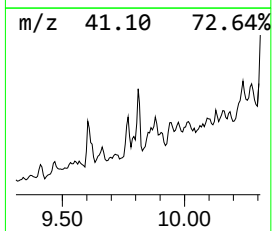
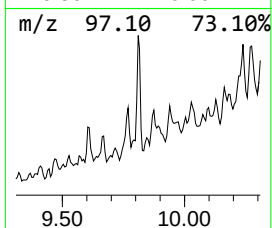
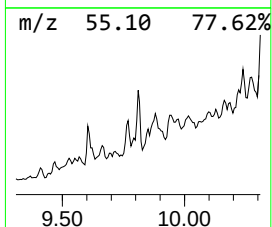
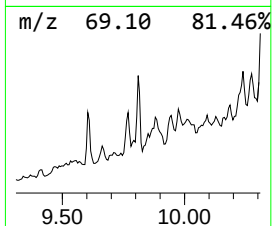
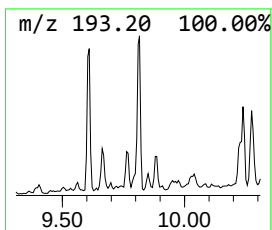
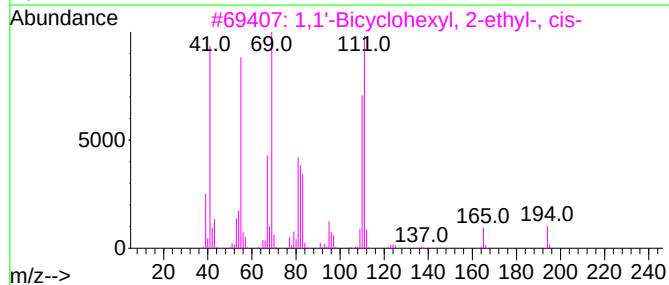
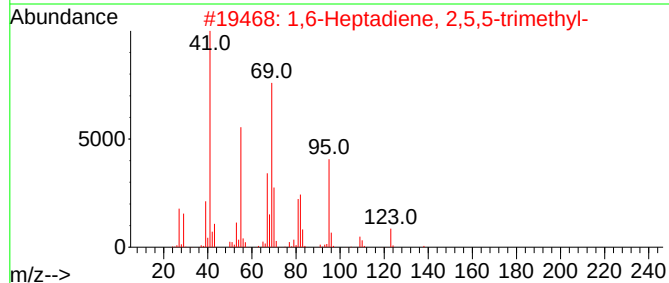
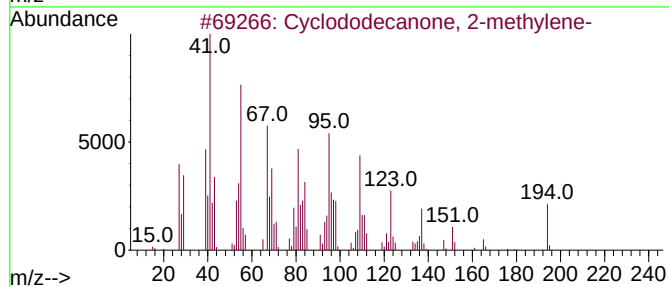
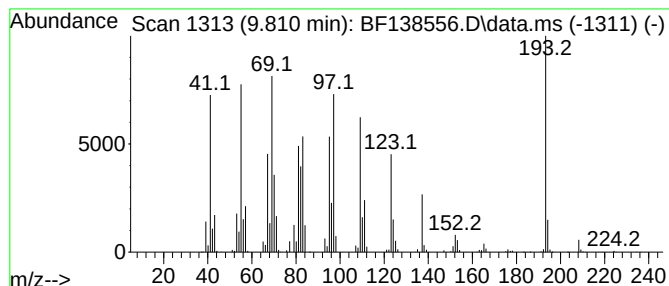
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.810 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.810	29.50 ng	1484270	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	25
2			1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	22
3			1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	20
4			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	18
5			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
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Sample : P3207-07
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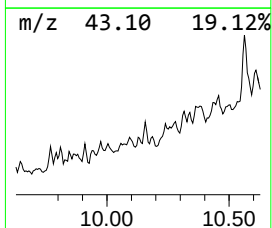
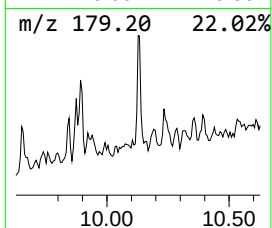
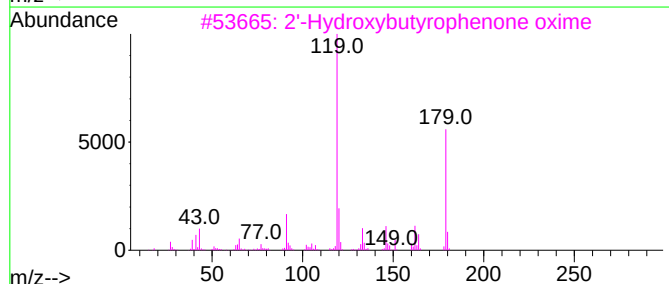
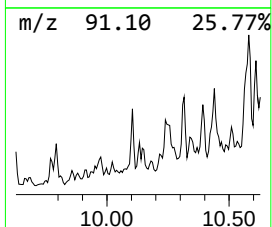
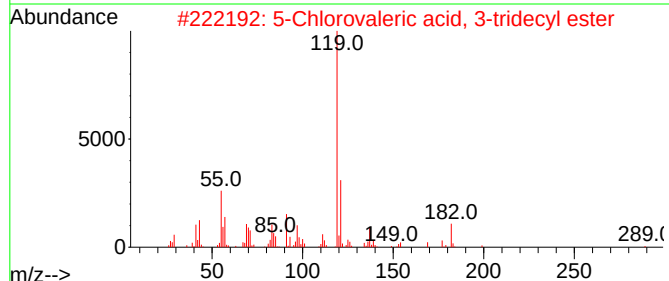
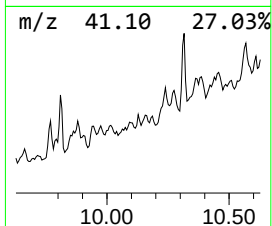
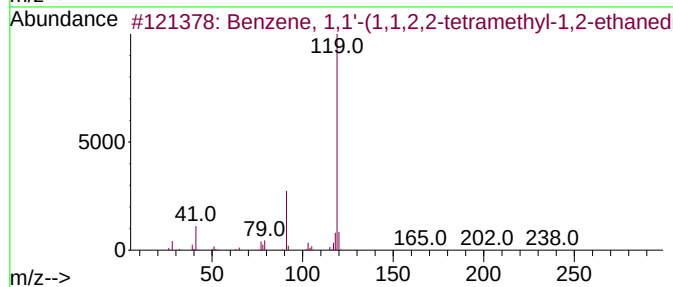
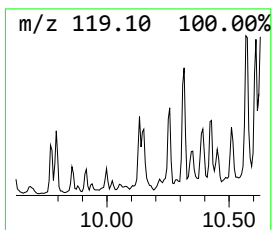
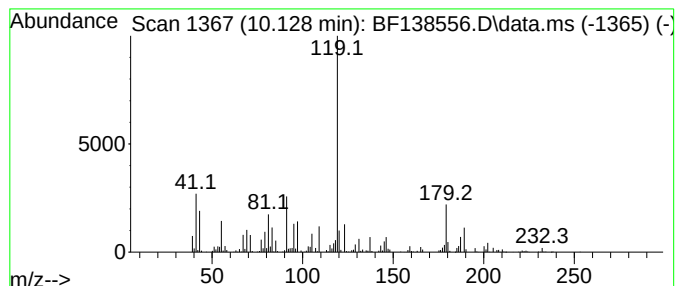
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.128 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.128	9.27 ng	466352	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	49
2			5-Chlorovaleric acid, 3-tridecyl...	318	C18H35ClO2	1000299-91-3	47
3			2'-Hydroxybutyrophenone oxime	179	C10H13NO2	021667-43-6	47
4			Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	46
5			2,4,4,6-Tetramethyl-6-phenylheptane	232	C17H28	1010293-28-6	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
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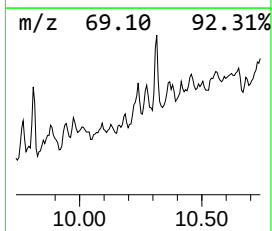
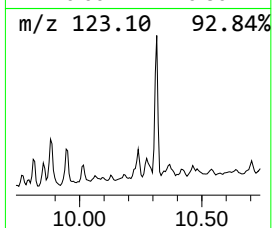
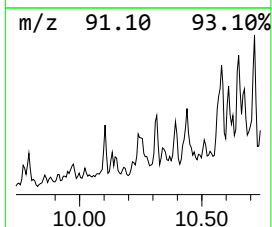
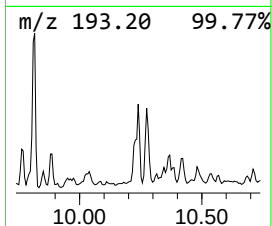
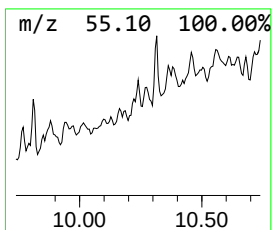
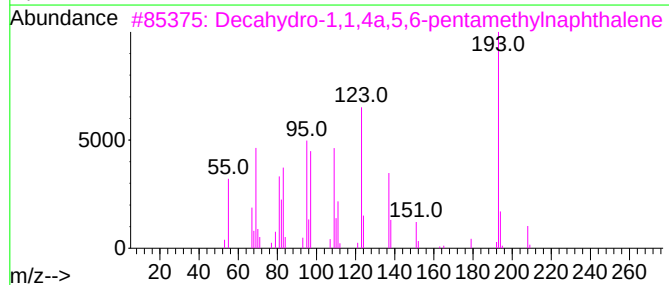
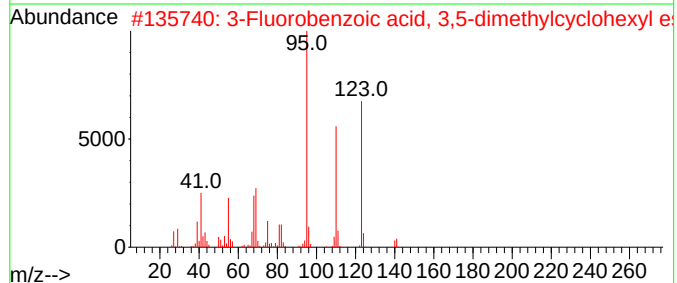
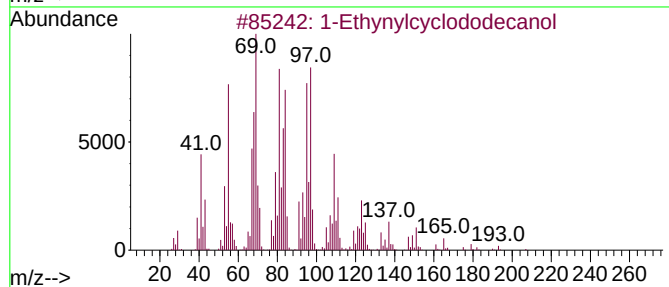
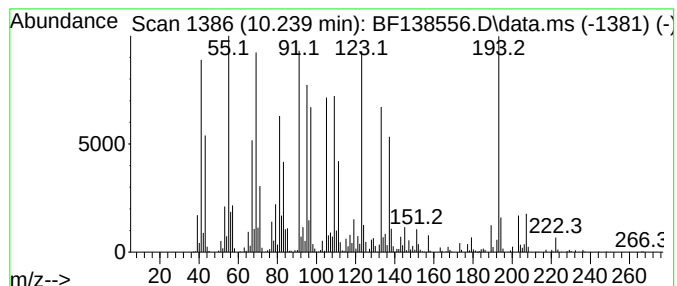
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Ethynylcyclododecanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.239	50.35 ng	2533350	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	60
2			3-Fluorobenzoic acid, 3,5-dimeth...	250	C15H19F02	1000279-01-8	38
3			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	27
4			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
5			(2E)-2-Heptylidene cyclohexanone	194	C13H22O	173975-69-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
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Misc :
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ClientSampleId :
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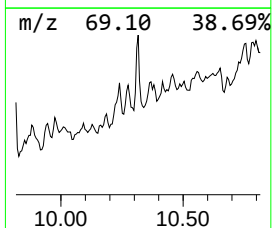
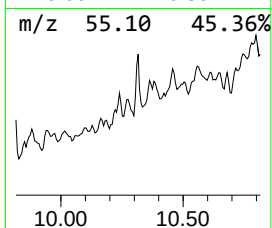
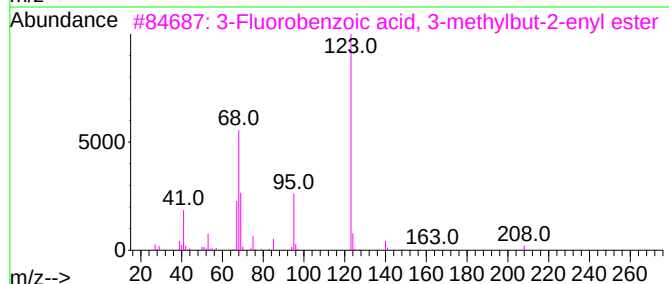
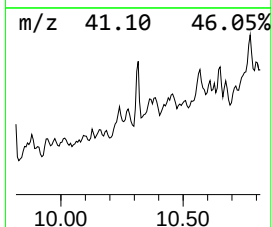
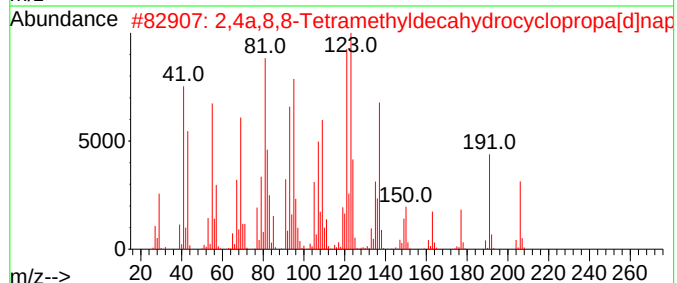
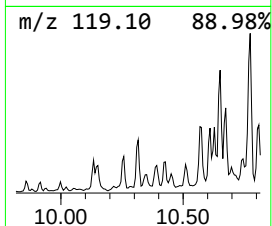
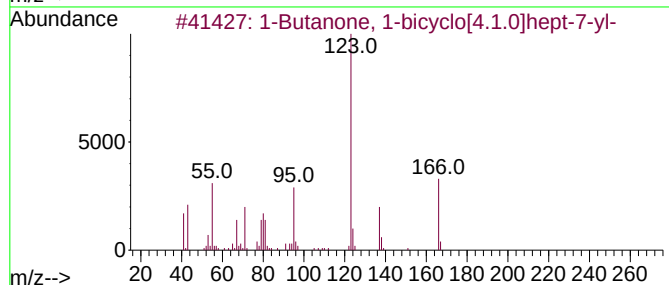
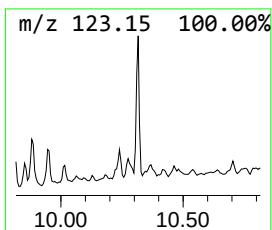
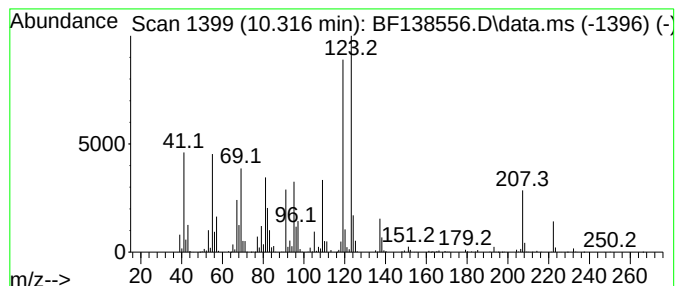
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.316 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	45.12 ng	2270340	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	35
2			2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	30
3			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	30
4			2-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000278-98-1	27
5			4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
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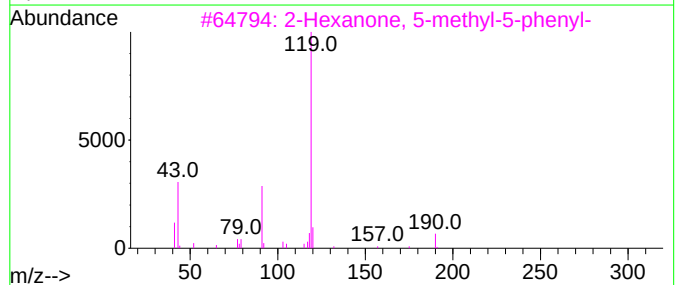
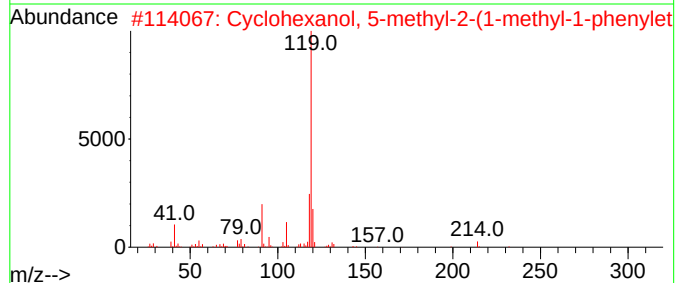
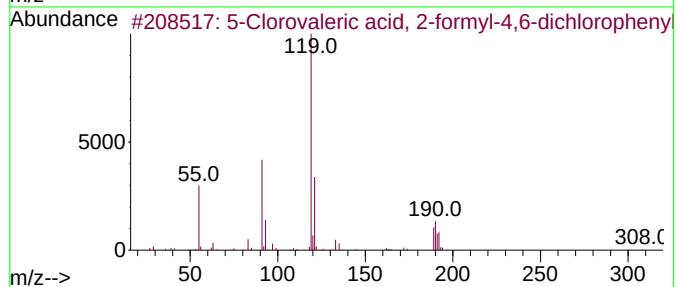
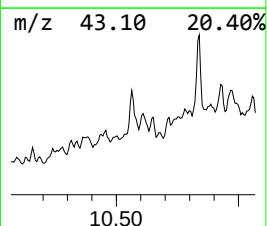
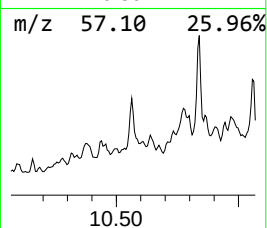
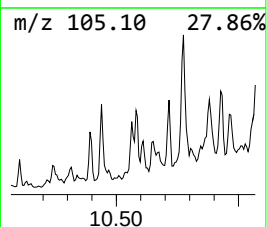
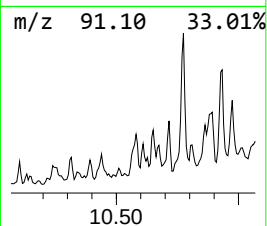
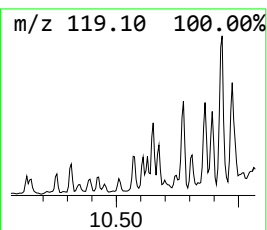
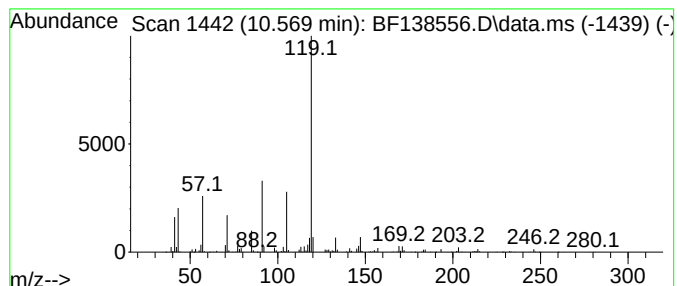
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 5-Clorovaleric acid, 2-form... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	36.29 ng	1826190	Acenaphthene-d10	9.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Clorovaleric acid, 2-formyl-4,...	308	C12H11Cl3O3	1000331-38-0	50
2		Cyclohexanol, 5-methyl-2-(1-meth...	232	C16H24O	134256-18-1	50
3		2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	50
4		p-Toluic acid, 2-chlorophenyl ester	246	C14H11ClO2	1000292-64-3	47
5		2,5-Pyrrolidinone, 1-[(3-methylb...	233	C12H11NO4	110920-15-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
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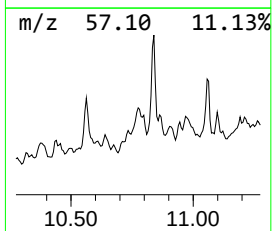
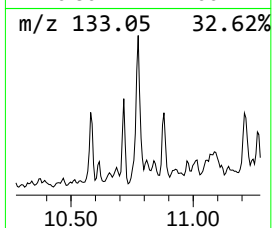
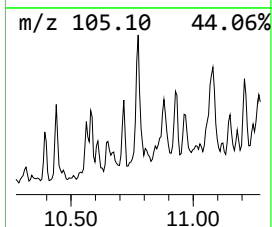
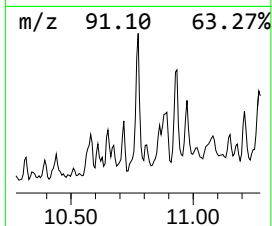
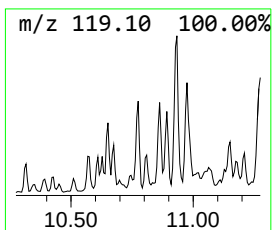
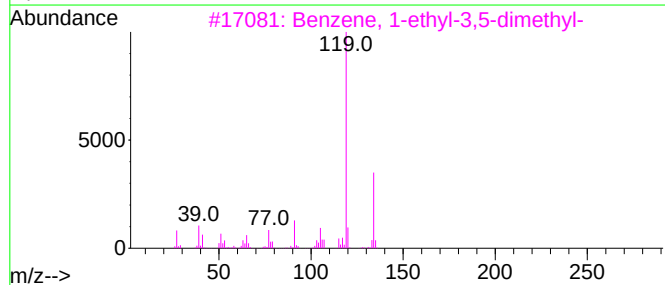
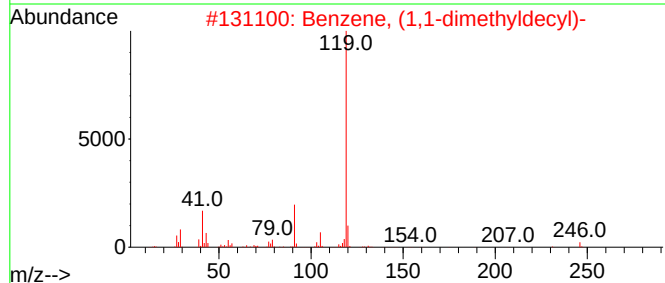
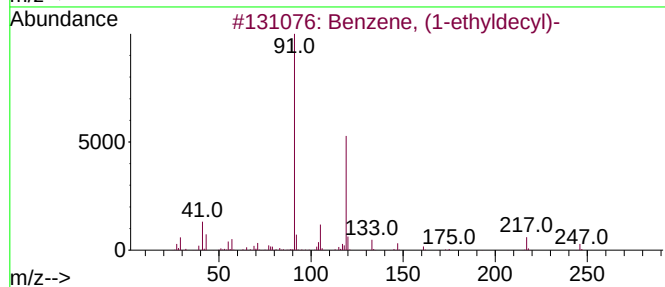
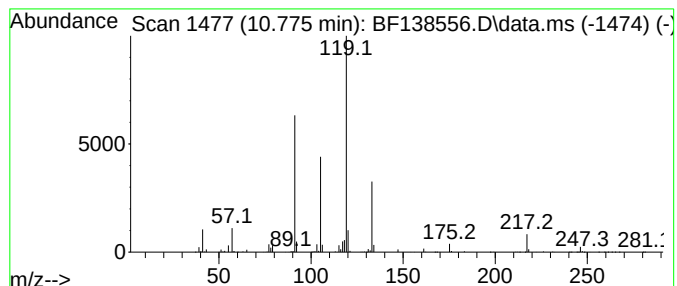
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzene, (1-ethyldecyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	30.83 ng	2374040	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	72
2			Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	62
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	59
4			Benzene, (1-ethylnonyl)-	232	C17H28	004536-87-2	59
5			Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
Operator : CG\JU
Sample : P3207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

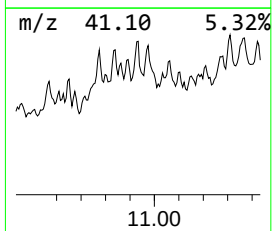
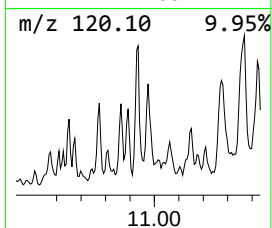
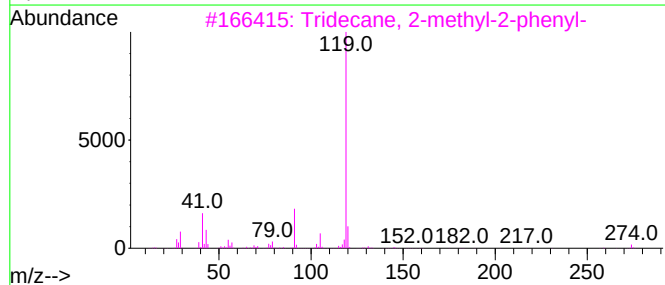
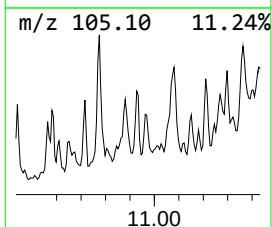
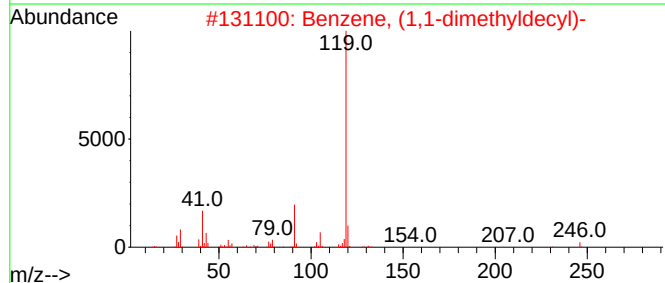
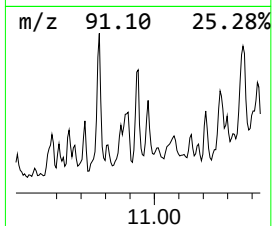
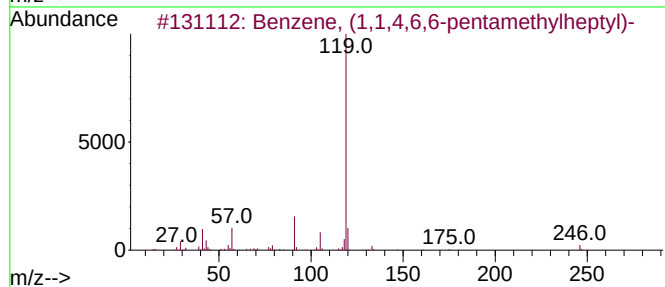
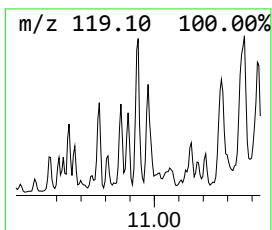
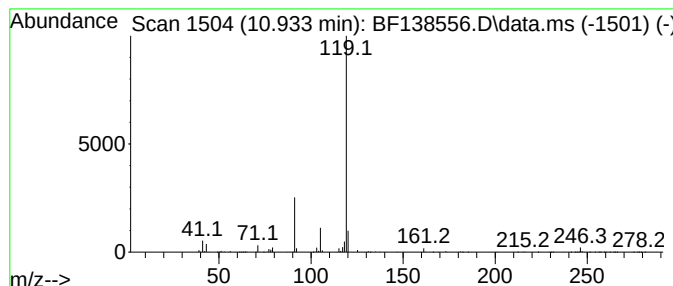
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzene, (1,1,4,6,6-pentame... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.933	23.80 ng	1832860	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, (1,1,4,6,6-pentamethylh...		246	C18H30	055134-07-1	91
2	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	91
3	Tridecane, 2-methyl-2-phenyl-		274	C20H34	027854-41-7	78
4	Pentadecane, 2-methyl-2-phenyl-		302	C22H38	029138-94-1	78
5	2-Hexanone, 5-methyl-5-phenyl-		190	C13H18O	014128-61-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
Operator : CG\JU
Sample : P3207-07
Misc :
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Instrument :
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ClientSampleId :
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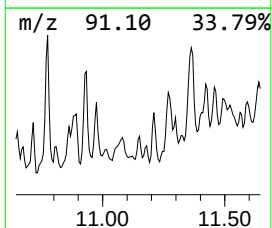
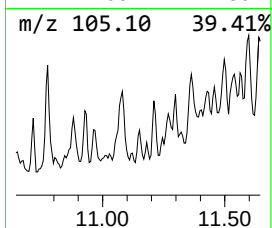
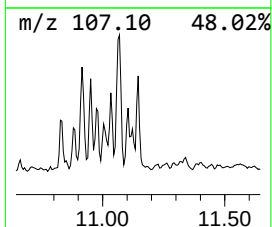
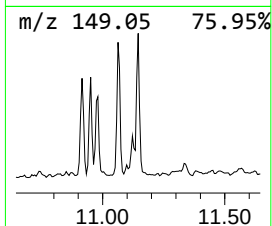
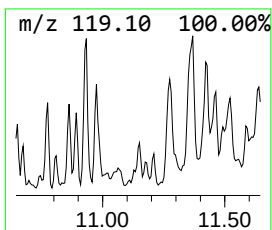
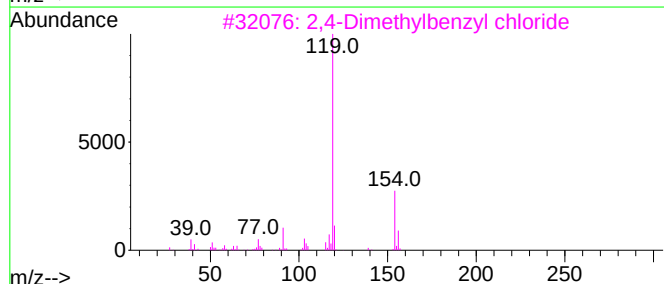
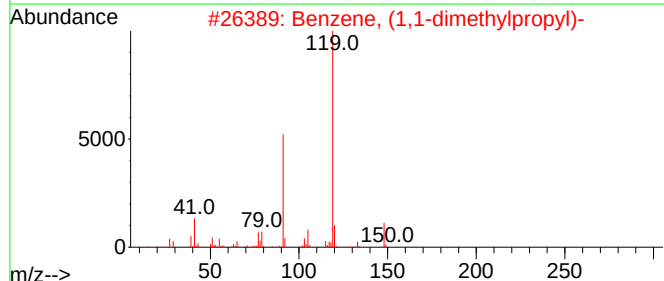
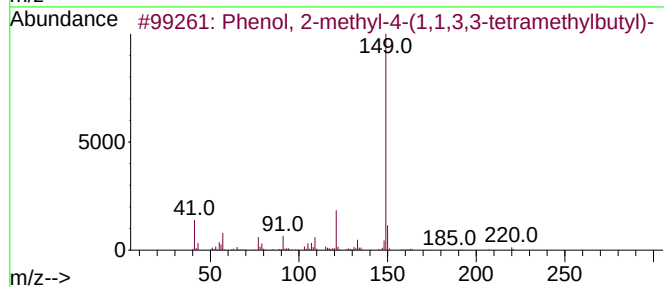
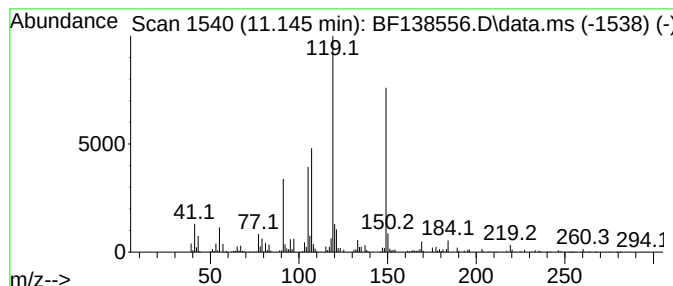
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown11.145 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.145	20.00 ng	1539910	Phenanthrene-d10	11.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	30
2		Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	27
3		2,4-Dimethylbenzyl chloride	154	C9H11Cl	000824-55-5	25
4		p-Toluic acid, oct-3-en-2-yl ester	246	C16H22O2	1000292-50-5	25
5		1,2-Benzenedicarboxylic acid, mo...	292	C17H24O4	024539-59-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
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Sample : P3207-07
Misc :
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ClientSampleId :
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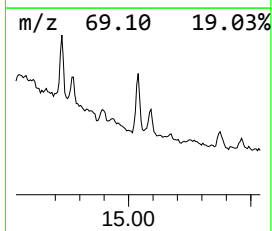
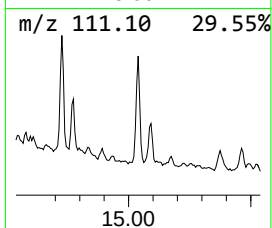
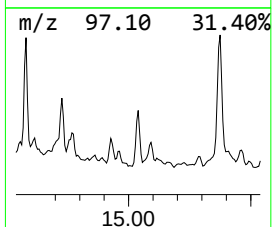
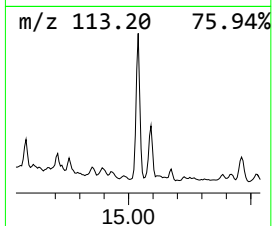
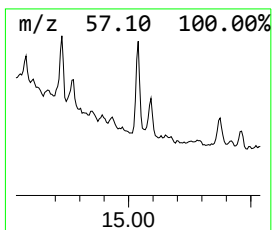
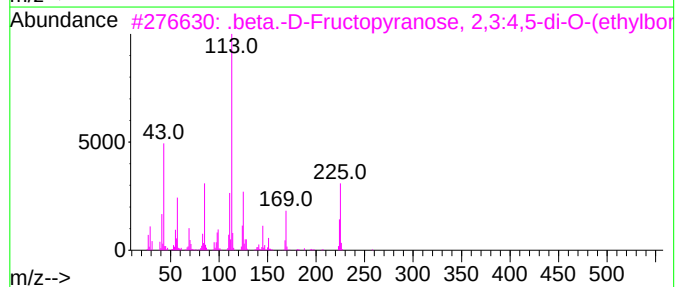
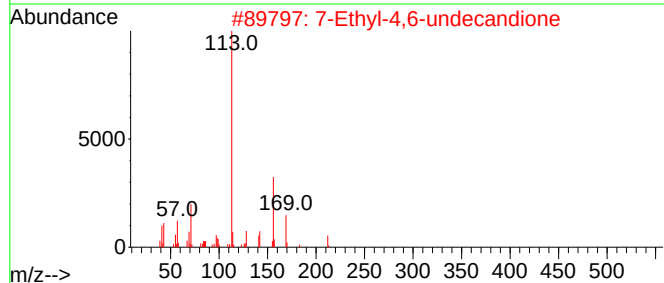
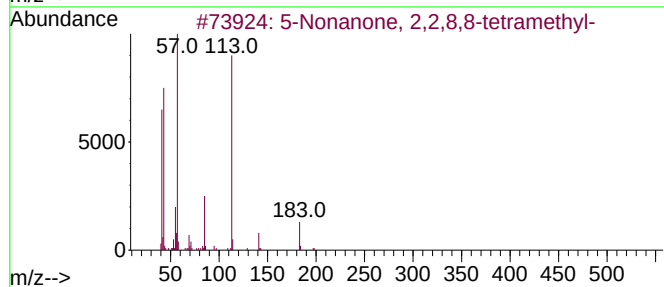
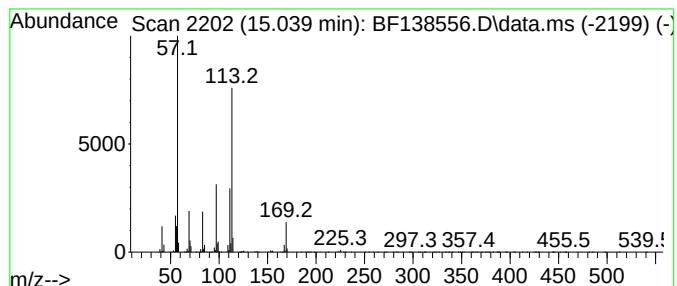
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown15.039 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.039	30.45 ng	1802630	Perylene-d12	15.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	47	
2	7-Ethyl-4,6-undecandione	212	C13H24O2	1000374-11-8	42	
3	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	42	
4	2,4,4-trimethylpentyl ethylphosp...	224	C10H22F02P	333416-13-0	40	
5	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	38	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
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Sample : P3207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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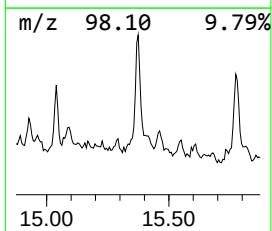
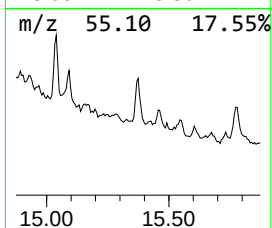
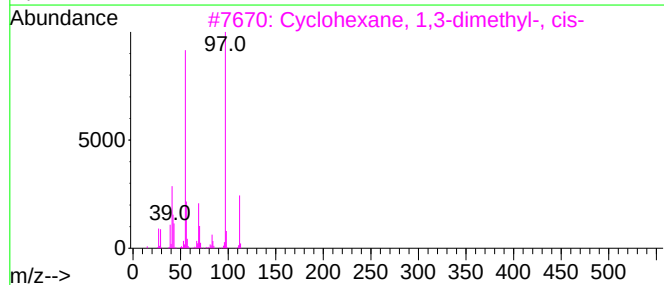
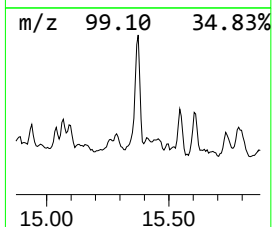
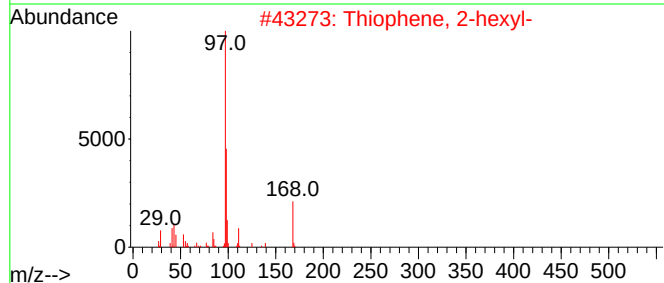
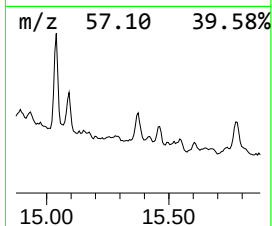
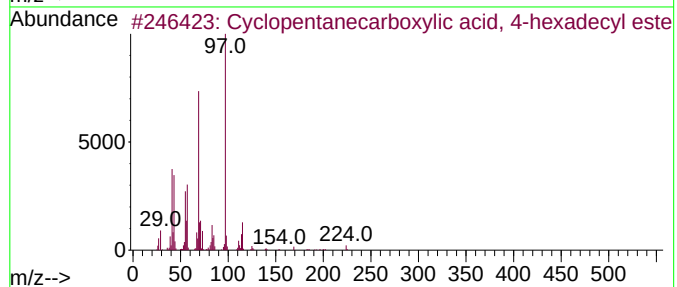
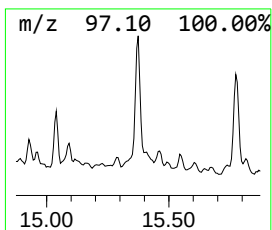
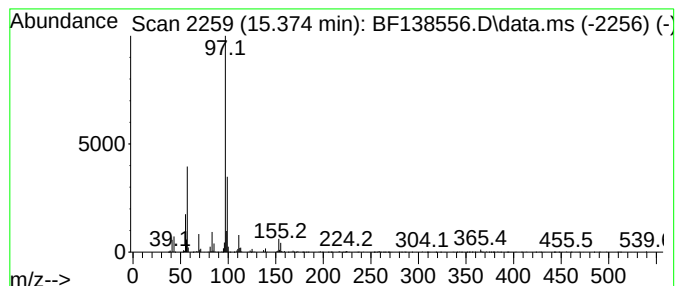
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Cyclopentanecarboxylic acid... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	20.00 ng	1183800	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	59
2			Thiophene, 2-hexyl-	168	C10H16S	018794-77-9	53
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	50
4			Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	50
5			Thiophene, 2-decyl-	224	C14H24S	024769-39-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
Operator : CG\JU
Sample : P3207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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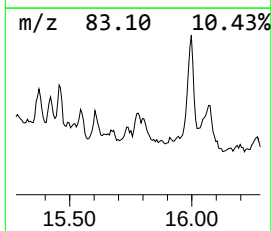
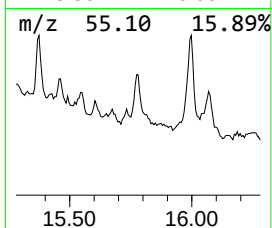
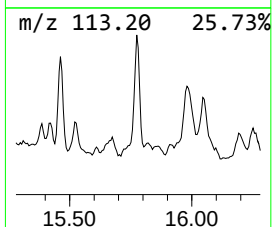
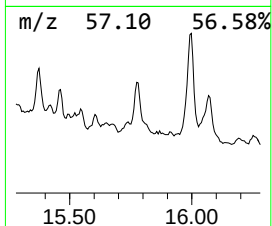
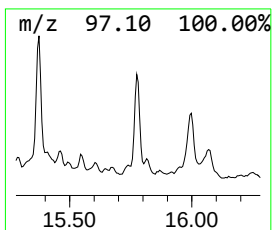
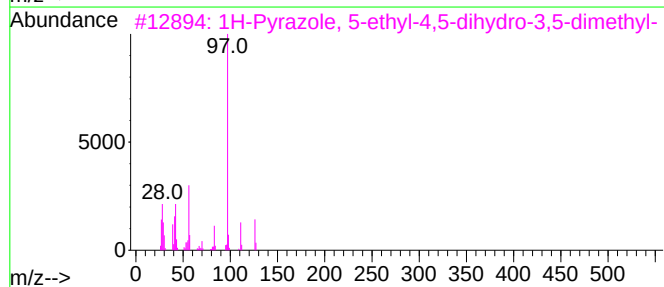
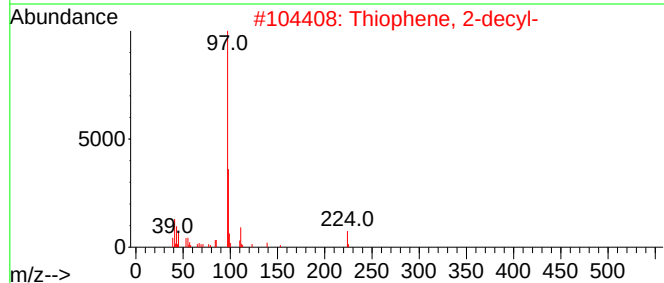
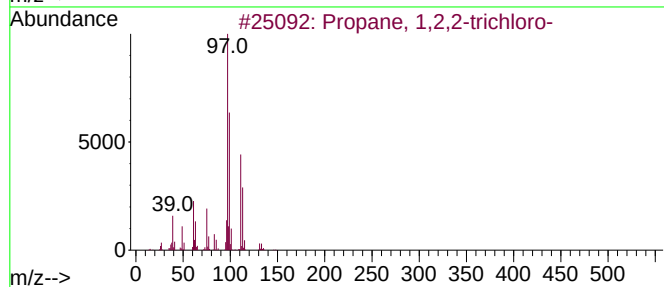
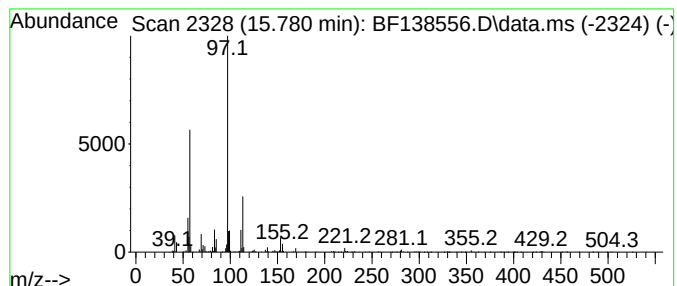
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Propane, 1,2,2-trichloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.780	29.81 ng	1764350	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,2,2-trichloro-	146	C3H5Cl3	003175-23-3	59
2			Thiophene, 2-decyl-	224	C14H24S	024769-39-9	52
3			1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	50
4			1H-Pyrazole-1-carboxamide, 4,5-d...	155	C7H13N3O	003786-02-5	50
5			1,1-Dimethyl-1-silacyclo-3-pentene	112	C6H12Si	016054-12-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
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Acq On : 12 Jul 2024 20:08
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Sample : P3207-07
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ALS Vial : 18 Sample Multiplier: 1

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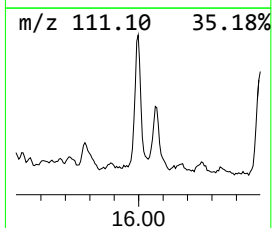
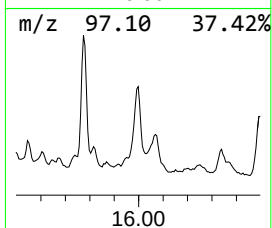
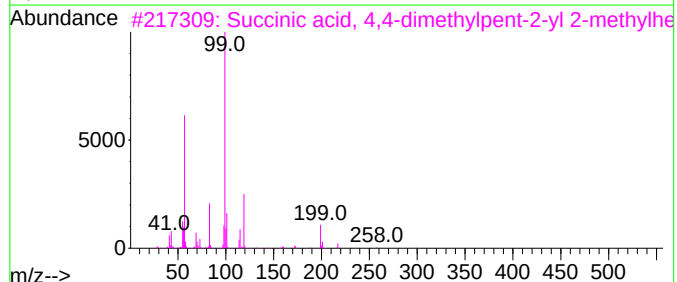
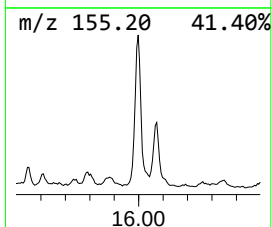
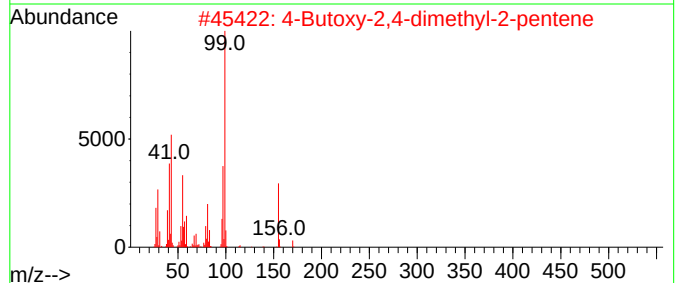
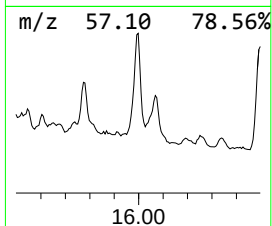
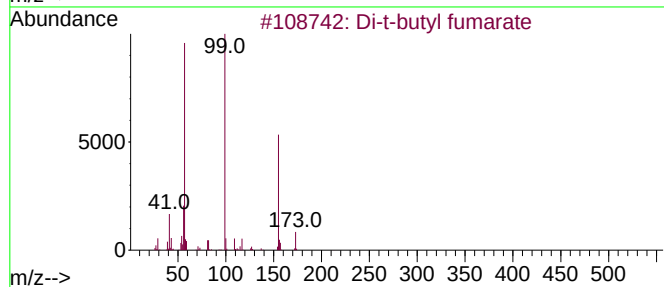
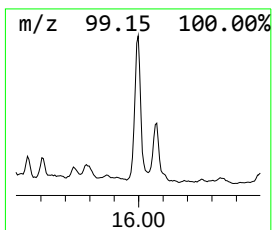
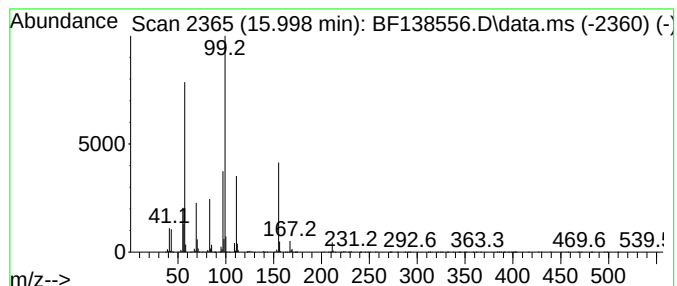
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Di-t-butyl fumarate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	42.19 ng	2497140	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-t-butyl fumarate	228	C12H20O4	007633-38-7	50
2			4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	50
3			Succinic acid, 4,4-dimethylpent-2-yl 2-methylhe	314	C18H34O4	1000381-71-8	37
4			d-glucose, 2-deoxy-3,5:4,6-di-O-...	240	C10H18B2O5	1000149-94-7	33
5			2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20F02P	333416-06-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
Operator : CG\JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RT-2929

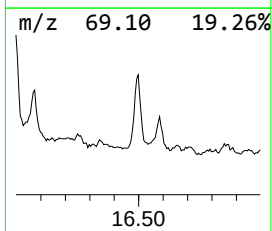
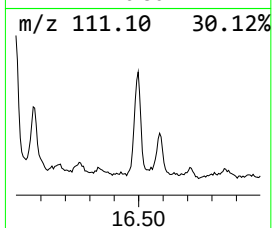
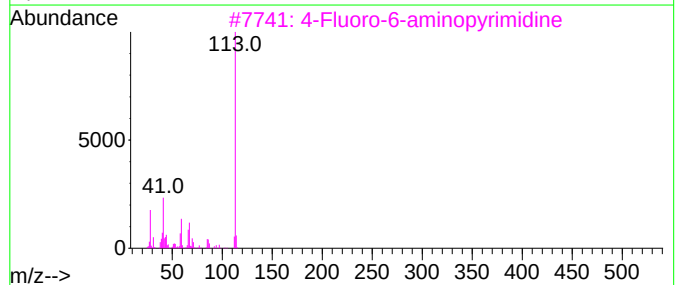
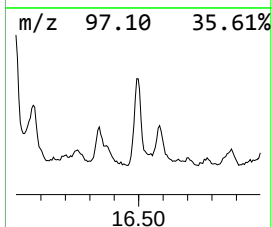
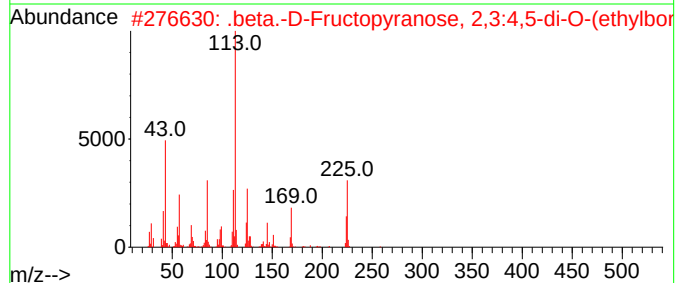
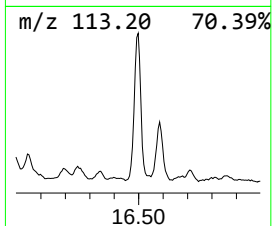
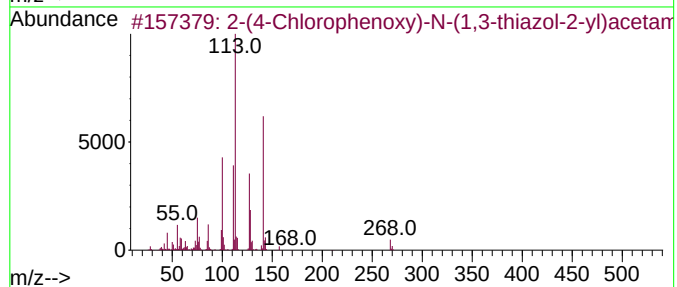
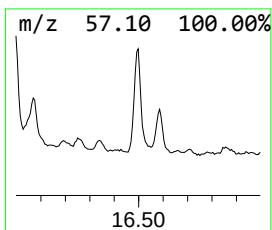
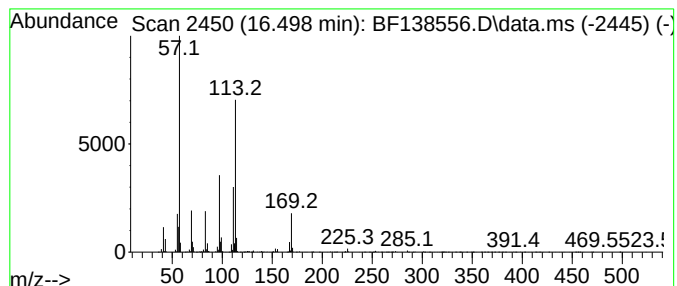
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown16.498 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.498	37.61 ng	2226070	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Chlorophenoxy)-N-(1,3-thiaz...	268	C11H9ClN2O2S	037666-22-1	38		
2	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	37		
3	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	30		
4	Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	27		
5	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
Operator : CG\JU
Sample : P3207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2929

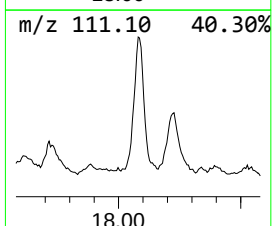
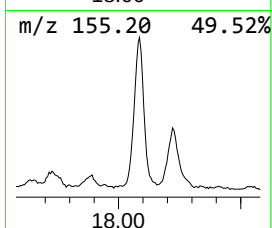
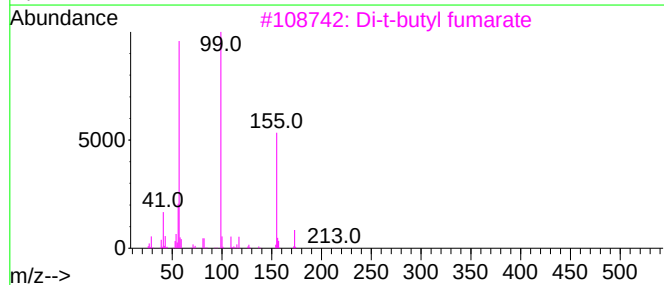
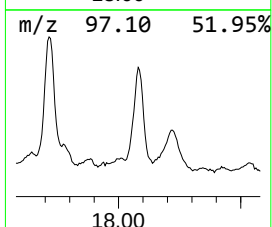
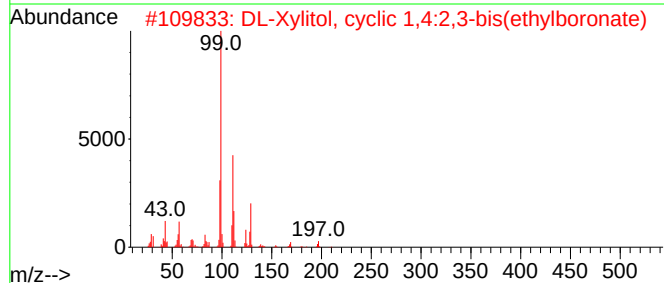
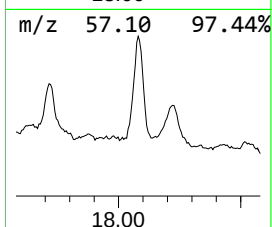
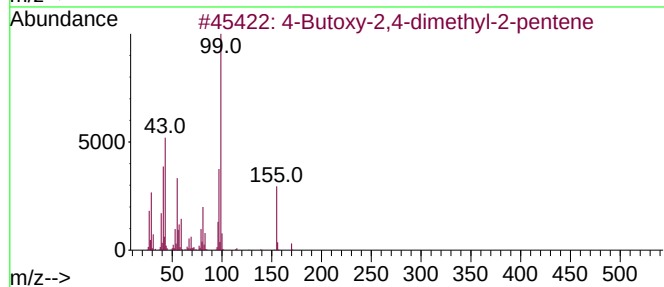
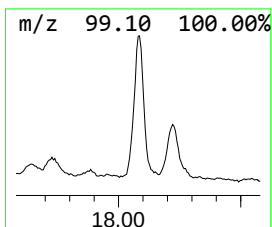
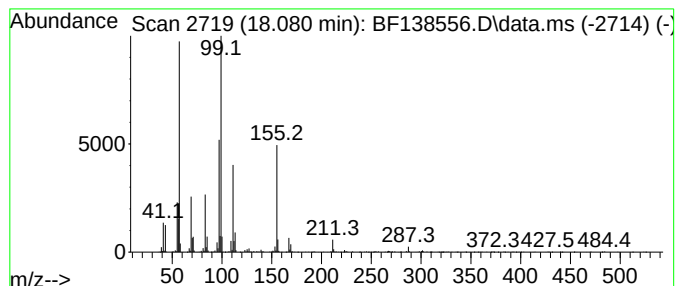
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown18.080 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.080	46.73 ng	2766200	Perylene-d12	15.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	38
2		DL-Xylitol, cyclic 1,4:2,3-bis(e...	228	C9H18B2O5	074793-31-0	38
3		Di-t-butyl fumarate	228	C12H20O4	007633-38-7	37
4		Fumaric acid, 2,4,4-trimethylpen...	372	C18H22Cl2O4	1000405-61-1	37
5		Fumaric acid, 2,4,4-trimethylpen...	342	C15H22F4O4	1000405-59-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138556.D
Acq On : 12 Jul 2024 20:08
Operator : CG\JU
Sample : P3207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2929

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
1-Nonene	8.075	111.3	ng	3075270	2	8.145	552527	20.0
(6-Chloro-2-met...	8.892	7.9	ng	219028	2	8.145	552527	20.0
Benzene, (1,1-d...	9.469	10.8	ng	545293	3	9.898	1006320	20.0
unknown9.604	9.604	35.8	ng	1798910	3	9.898	1006320	20.0
unknown9.769	9.769	25.2	ng	1268060	3	9.898	1006320	20.0
Benzene, 1,1'-(...	9.792	11.9	ng	597781	3	9.898	1006320	20.0
unknown9.810	9.810	29.5	ng	1484270	3	9.898	1006320	20.0
unknown10.128	10.128	9.3	ng	466352	3	9.898	1006320	20.0
1-Ethynylcyclo...	10.239	50.4	ng	2533350	3	9.898	1006320	20.0
unknown10.316	10.316	45.1	ng	2270340	3	9.898	1006320	20.0
5-Chlorovaleric ...	10.569	36.3	ng	1826190	3	9.898	1006320	20.0
Benzene, (1-eth...	10.775	30.8	ng	2374040	4	11.410	1539910	20.0
Benzene, (1,1,4...	10.933	23.8	ng	1832860	4	11.410	1539910	20.0
unknown11.145	11.145	20.0	ng	1539910	4	11.410	1539910	20.0
unknown15.039	15.039	30.4	ng	1802630	6	15.539	1183800	20.0
Cyclopentanecar...	15.374	20.0	ng	1183800	6	15.539	1183800	20.0
Propane, 1,2,2-...	15.780	29.8	ng	1764350	6	15.539	1183800	20.0
Di-t-butyl fuma...	15.998	42.2	ng	2497140	6	15.539	1183800	20.0
unknown16.498	16.498	37.6	ng	2226070	6	15.539	1183800	20.0
unknown18.080	18.080	46.7	ng	2766200	6	15.539	1183800	20.0