

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091622\
 Data File : BF130295.D
 Acq On : 16 Sep 2022 17:47
 Operator : CG\JU
 Sample : N4663-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HW-43

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130295.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.840	465	468	478	rVB	101620	111690	4.03%	0.748%
2	5.263	535	540	543	rBV	945958	891054	32.17%	5.964%
3	6.293	711	715	719	rBV	703820	595791	21.51%	3.988%
4	6.328	719	721	726	rVB	68691	60710	2.19%	0.406%
5	6.669	775	779	782	rBV	582058	513873	18.55%	3.439%
6	7.234	870	875	878	rVB	1665643	1566620	56.55%	10.486%
7	7.440	905	910	913	rVB4	29180	35083	1.27%	0.235%
8	7.945	992	996	999	rBV	782095	673822	24.32%	4.510%
9	8.022	1006	1009	1015	rVB	89759	79936	2.89%	0.535%
10	8.422	1067	1077	1080	rBV7	37082	66478	2.40%	0.445%
11	8.787	1134	1139	1145	rVB5	40030	64045	2.31%	0.429%
12	9.028	1175	1180	1183	rBV	3249030	2770183	100.00%	18.542%
13	9.169	1195	1204	1207	rBV	35081	46812	1.69%	0.313%
14	9.357	1233	1236	1239	rBV3	27438	35519	1.28%	0.238%
15	9.475	1253	1256	1257	rBV2	60019	54260	1.96%	0.363%
16	9.557	1266	1270	1279	rBV	68979	64062	2.31%	0.429%
17	9.698	1288	1294	1296	rBV	853618	716654	25.87%	4.797%
18	9.728	1296	1299	1303	rVB	696023	554513	20.02%	3.712%
19	9.898	1325	1328	1332	rVV	35942	36884	1.33%	0.247%
20	9.939	1332	1335	1339	rVB	39782	33297	1.20%	0.223%
21	10.016	1344	1348	1350	rBV	77686	79760	2.88%	0.534%
22	10.092	1358	1361	1364	rBV2	36957	46811	1.69%	0.313%
23	10.122	1364	1366	1370	rVB2	51416	45395	1.64%	0.304%
24	10.239	1382	1386	1389	rVB2	168003	147709	5.33%	0.989%
25	10.310	1389	1398	1399	rBV2	63130	74649	2.69%	0.500%
26	10.398	1410	1413	1418	rVB3	34246	48657	1.76%	0.326%
27	10.481	1423	1427	1432	rBV	1214522	987676	35.65%	6.611%
28	10.604	1446	1448	1453	rVB	31224	31138	1.12%	0.208%
29	10.675	1456	1460	1463	rBV3	26196	35932	1.30%	0.241%
30	10.781	1473	1478	1481	rBV3	24145	35184	1.27%	0.235%
31	10.933	1499	1504	1510	rVB6	17674	34196	1.23%	0.229%
32	11.175	1541	1545	1548	rBV	738056	573117	20.69%	3.836%
33	11.716	1633	1637	1641	rBV	75535	85282	3.08%	0.571%
34	12.516	1765	1773	1782	rBV	1220018	1176363	42.47%	7.874%
35	12.763	1810	1815	1818	rBV	1978738	1694651	61.17%	11.343%
36	12.927	1840	1843	1847	rVB	63382	58001	2.09%	0.388%

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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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.804	1988	1992	1995	rBV	397106	372239	13.44%	2.491%
38	15.192	2223	2228	2233	rBV	404245	442353	15.97%	2.961%

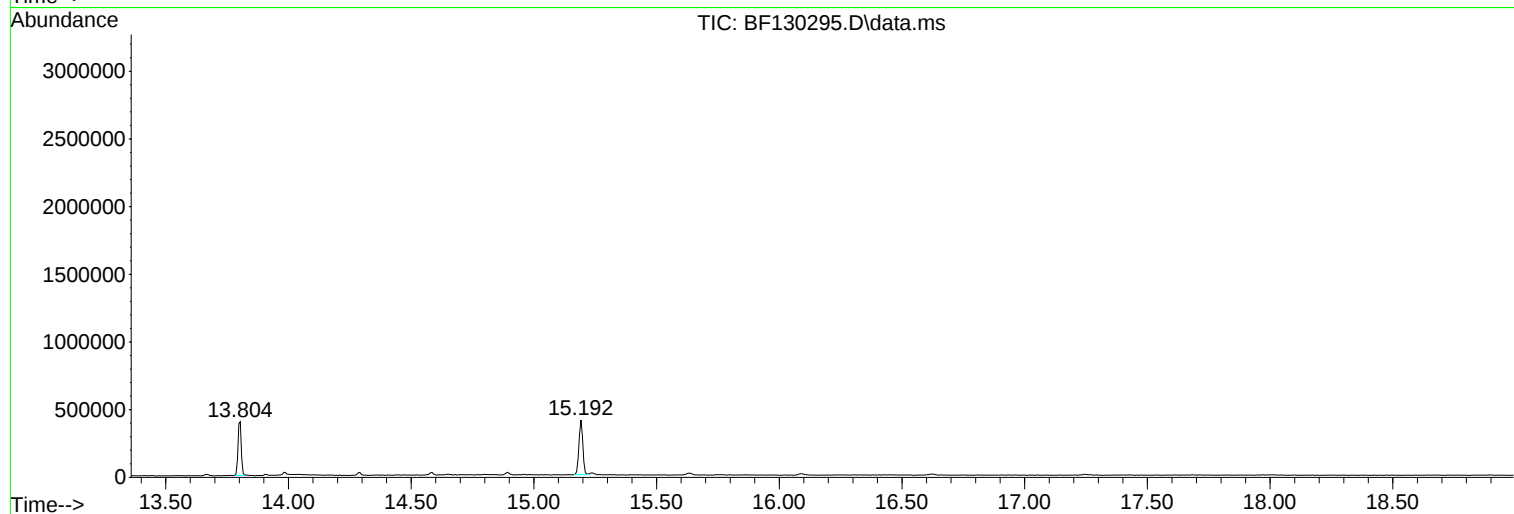
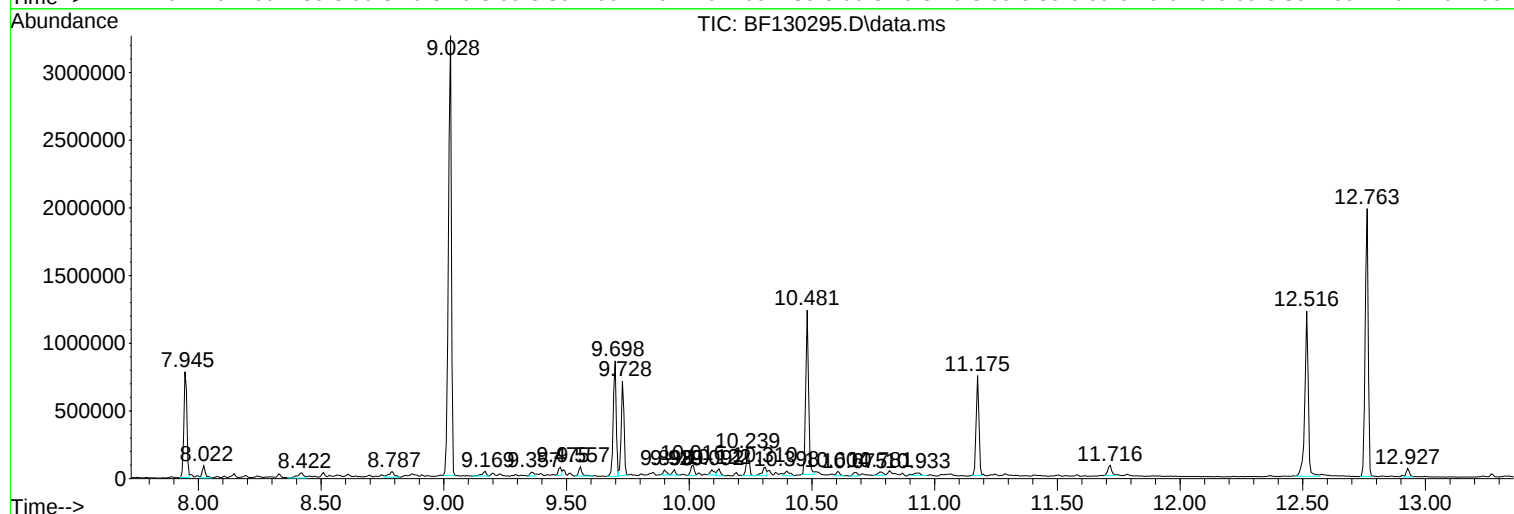
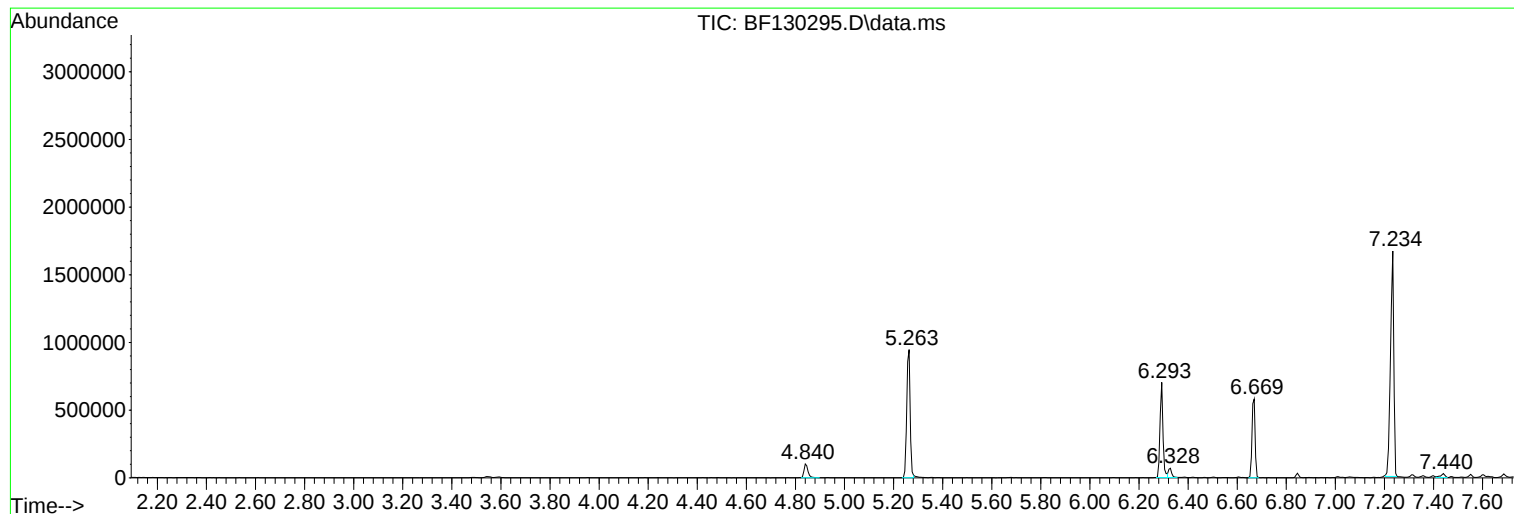
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
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Instrument :
BNA_F
ClientSampleId :
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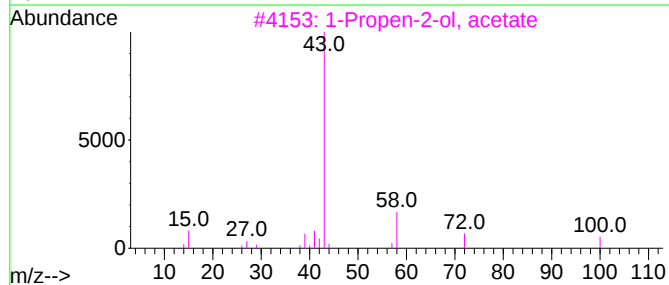
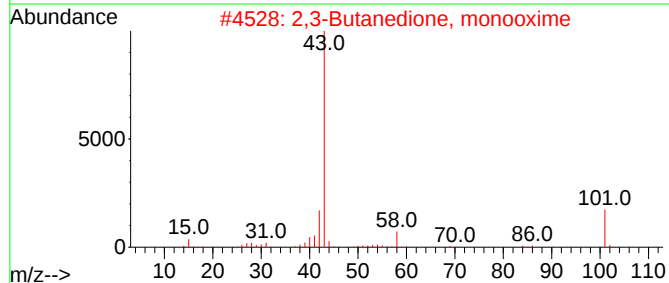
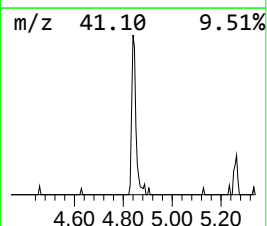
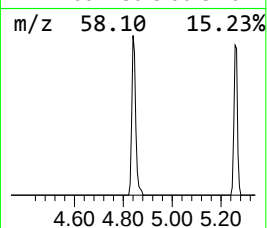
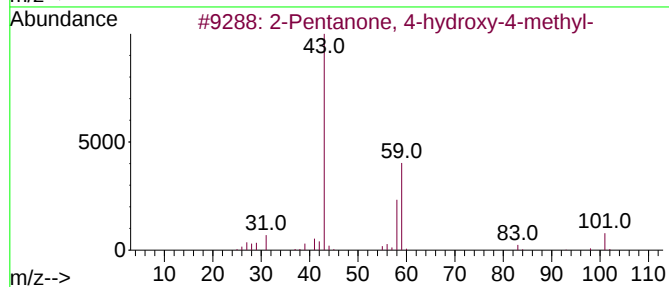
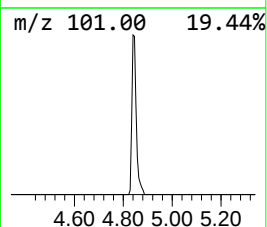
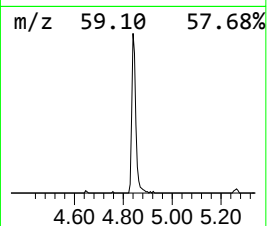
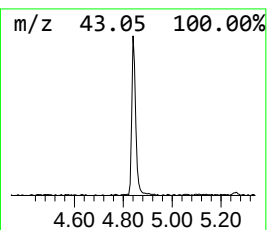
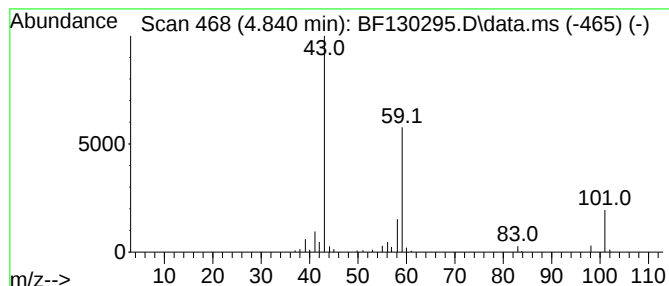
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.840	4.35 ng	111690	1,4-Dichlorobenzene-d4	6.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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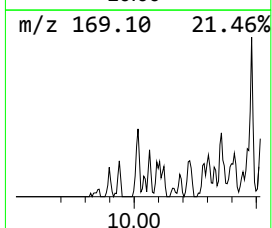
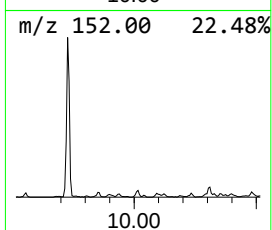
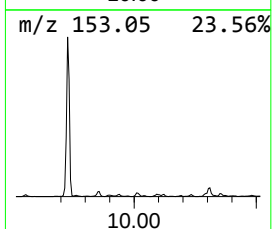
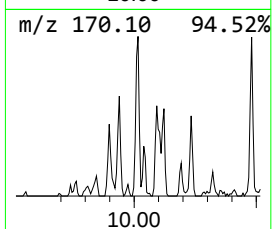
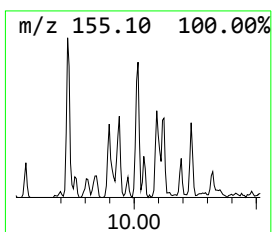
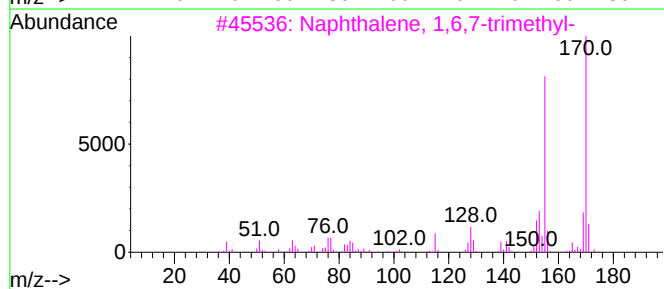
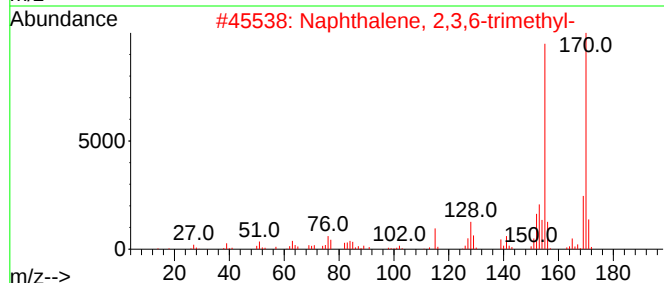
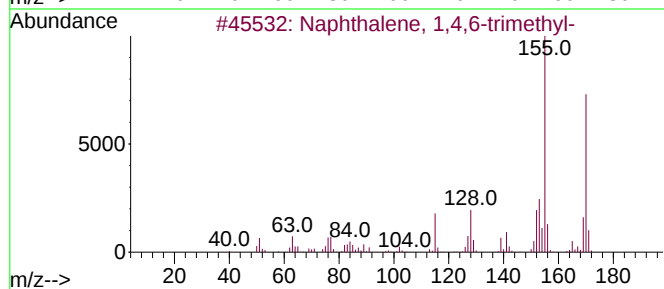
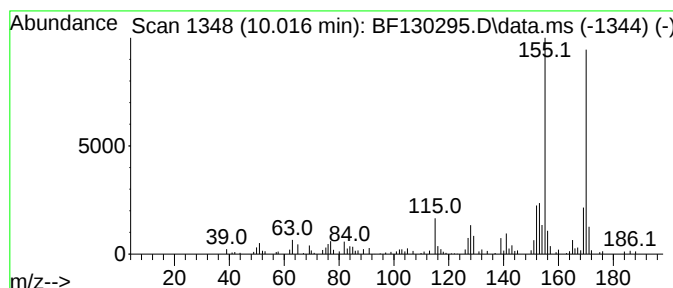
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, 1,4,6-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.016	2.23 ng	79760	Acenaphthene-d10	9.698	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	97
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	97
3	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	97
4	1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	93
5	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	93



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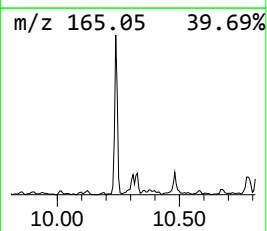
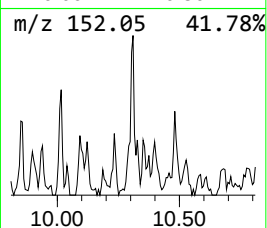
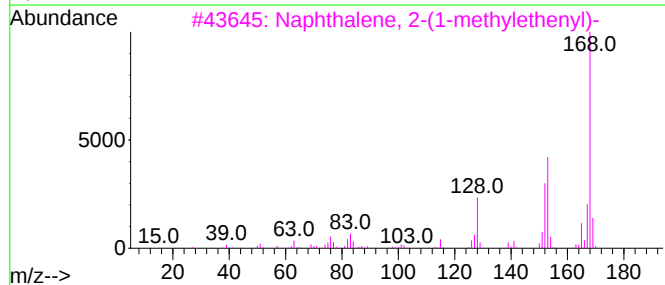
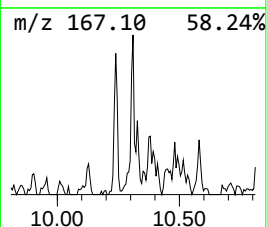
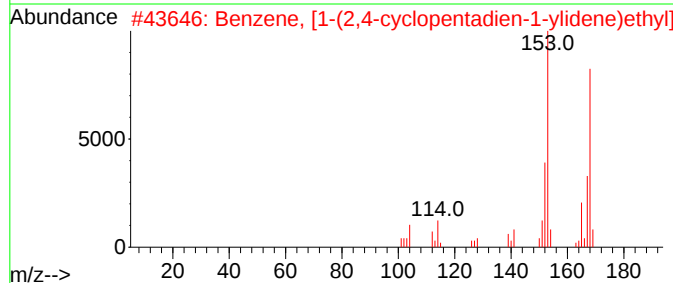
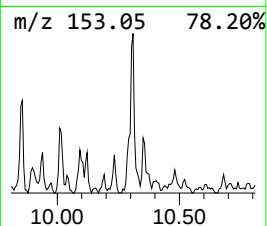
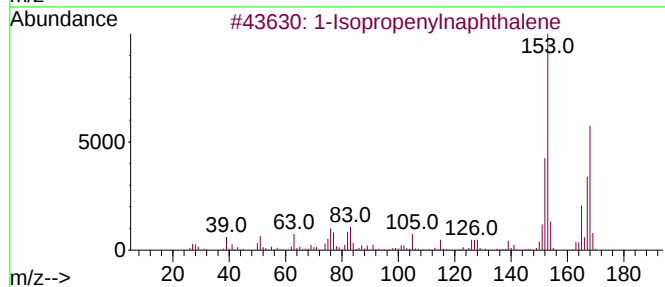
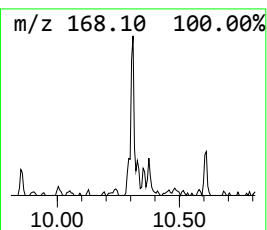
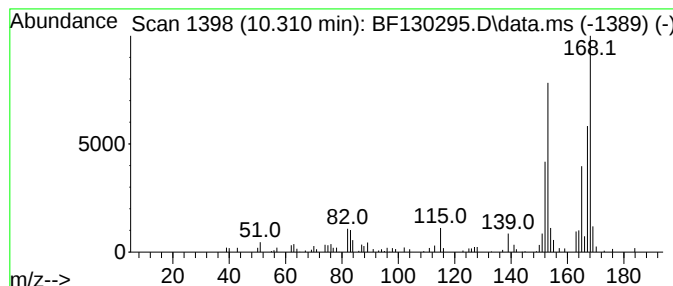
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Isopropenylnaphthalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.310	2.08 ng	74649	Acenaphthene-d10	9.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Isopropenylnaphthalene	168	C13H12	001855-47-6	76
2			Benzene, [1-(2,4-cyclopentadien-...	168	C13H12	002320-32-3	64
3			Naphthalene, 2-(1-methylethenyl)-	168	C13H12	003710-23-4	59
4			Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	53
5			1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	53



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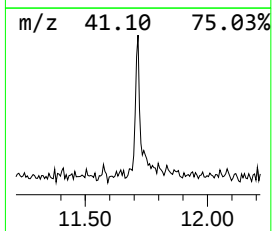
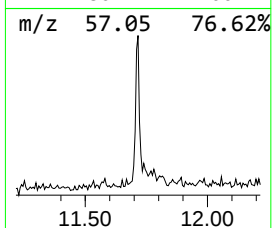
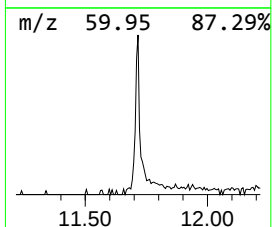
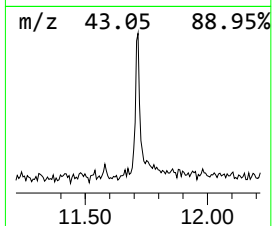
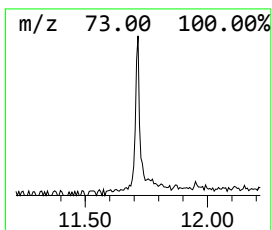
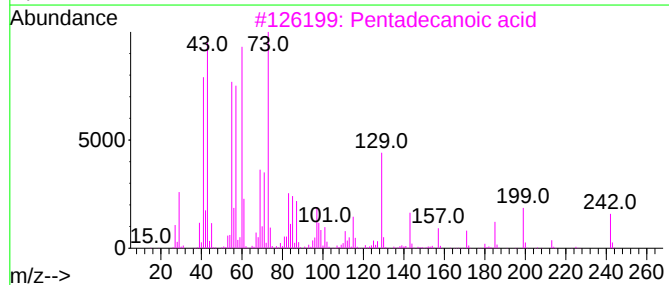
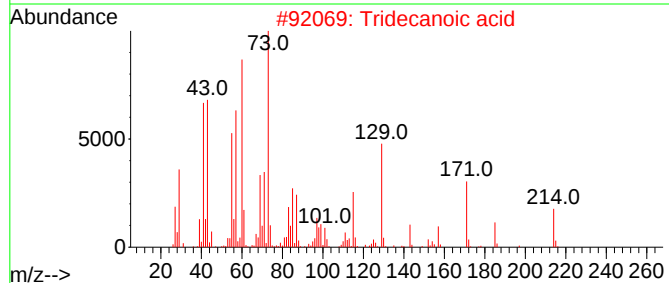
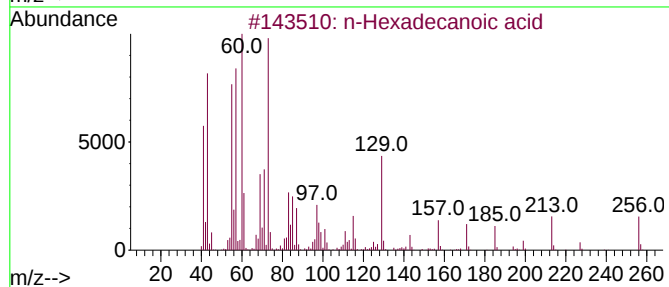
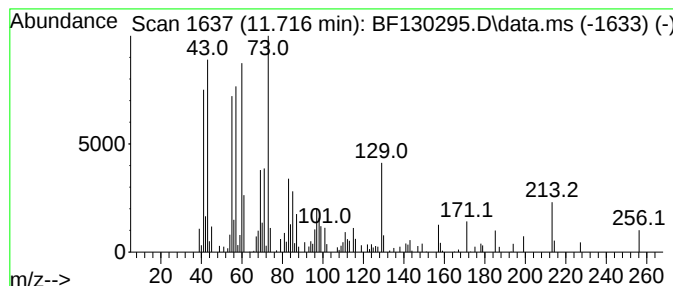
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	2.98 ng	85282	Phenanthrene-d10	11.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Acetamide, N-(4-hydroxycyclohexy...	157	C8H15NO2	027489-60-7	25



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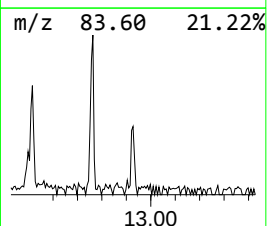
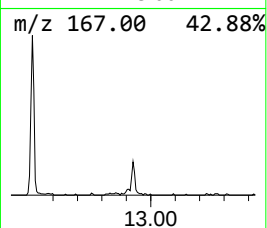
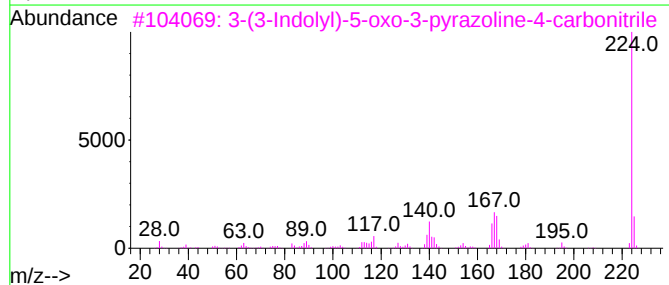
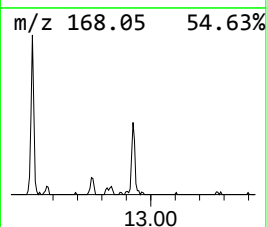
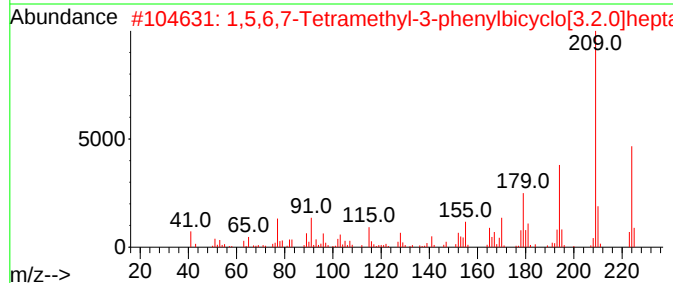
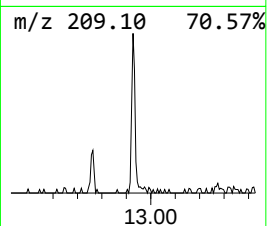
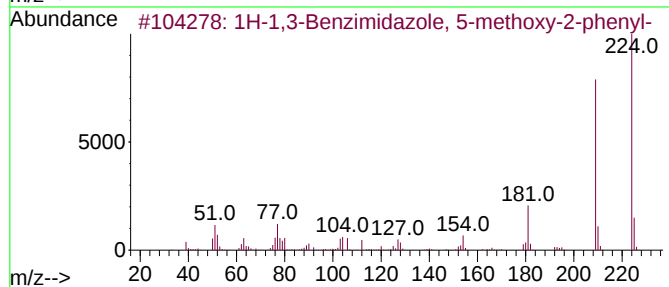
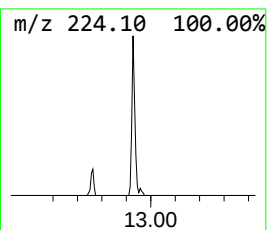
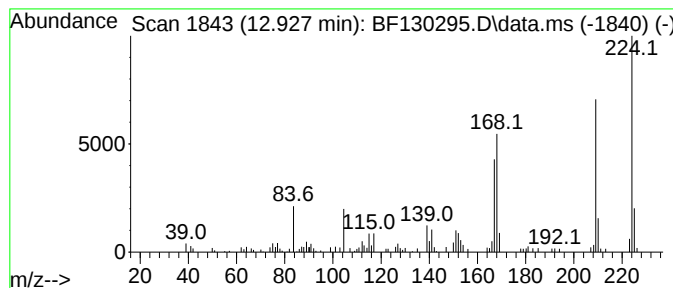
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown12.928 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.928	3.12 ng	58001	Chrysene-d12	13.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,3-Benzimidazole, 5-methoxy-...	224	C14H12N2O	1000350-62-4	49		
2	1,5,6,7-Tetramethyl-3-phenylbicy...	224	C17H20	126584-00-7	46		
3	3-(3-Indolyl)-5-oxo-3-pyrazoline...	224	C12H8N4O	1000240-73-4	45		
4	1H-Purine-2,6-dione, 3,7-dihydro...	224	C9H12N4O3	000569-34-6	43		
5	9,10-Anthracenedione, 1-hydroxy-	224	C14H8O3	000129-43-1	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091622\
Data File : BF130295.D
Acq On : 16 Sep 2022 17:47
Operator : CG\JU
Sample : N4663-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-43

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
2-Pentanone, 4-...	4.840	4.3	ng	111690	1	6.669	513873	20.0
Naphthalene, 1,...	10.016	2.2	ng	79760	3	9.698	716654	20.0
1-Isopropenylna...	10.310	2.1	ng	74649	3	9.698	716654	20.0
n-Hexadecanoic ...	11.716	3.0	ng	85282	4	11.175	573117	20.0
unknown12.928	12.928	3.1	ng	58001	5	13.804	372239	20.0