

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
 Data File : BF142647.D
 Acq On : 06 Jun 2025 15:29
 Operator : RC/JU
 Sample : Q2214-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR251425

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-BF052025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.104	485	495	503	rBV	125657	185043	10.87%	1.152%
2	5.510	558	564	569	rBV	1311439	1693264	99.47%	10.546%
3	6.516	729	735	751	rVB	1282695	1702204	100.00%	10.602%
4	6.892	794	799	804	rBV	583724	709632	41.69%	4.420%
5	7.451	885	894	904	rBV	818080	1117081	65.63%	6.957%
6	7.704	934	937	945	rVB2	15668	23472	1.38%	0.146%
7	8.181	1011	1018	1023	rBV	701627	948145	55.70%	5.905%
8	8.228	1023	1026	1030	rVB2	20825	26749	1.57%	0.167%
9	8.469	1064	1067	1071	rVB5	16812	21319	1.25%	0.133%
10	8.680	1100	1103	1106	rBV2	23570	29242	1.72%	0.182%
11	8.998	1154	1157	1160	rBV	50270	65631	3.86%	0.409%
12	9.139	1175	1181	1184	rBV5	42934	91589	5.38%	0.570%
13	9.251	1195	1200	1205	rBV	1233814	1535277	90.19%	9.562%
14	9.327	1209	1213	1217	rBV4	107523	162931	9.57%	1.015%
15	9.569	1250	1254	1255	rBV3	76193	92759	5.45%	0.578%
16	9.598	1255	1259	1263	rVB	201862	280741	16.49%	1.749%
17	9.645	1263	1267	1271	rBV3	173920	274525	16.13%	1.710%
18	9.804	1290	1294	1296	rBV3	127504	185657	10.91%	1.156%
19	9.845	1298	1301	1305	rVB2	196860	266618	15.66%	1.661%
20	9.933	1310	1316	1320	rVV	808204	1161389	68.23%	7.233%
21	10.345	1383	1386	1391	rBV2	198889	252260	14.82%	1.571%
22	10.727	1447	1451	1455	rBV	762401	1019550	59.90%	6.350%
23	10.851	1469	1472	1479	rVB	454972	634955	37.30%	3.955%
24	11.427	1567	1570	1575	rBV	634891	835047	49.06%	5.201%
25	13.010	1835	1839	1848	rVB	758046	1042553	61.25%	6.493%
26	14.068	2014	2019	2032	rVB	469160	699172	41.07%	4.355%
27	14.551	2098	2101	2115	rVB2	66856	114131	6.70%	0.711%
28	14.992	2173	2176	2184	rVB6	17980	27774	1.63%	0.173%
29	15.121	2194	2198	2205	rVB	17850	37053	2.18%	0.231%
30	15.192	2206	2210	2214	rBV	20165	30811	1.81%	0.192%
31	15.562	2267	2273	2291	rVB	452285	749330	44.02%	4.667%
32	16.033	2348	2353	2359	rBV	22590	40129	2.36%	0.250%

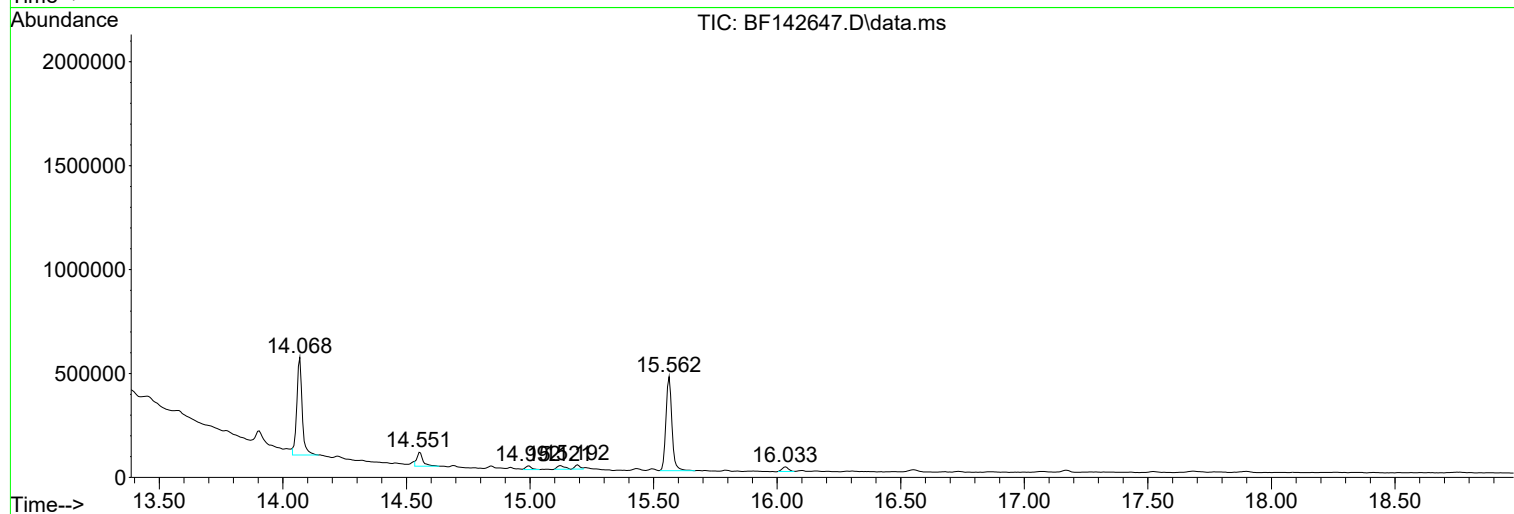
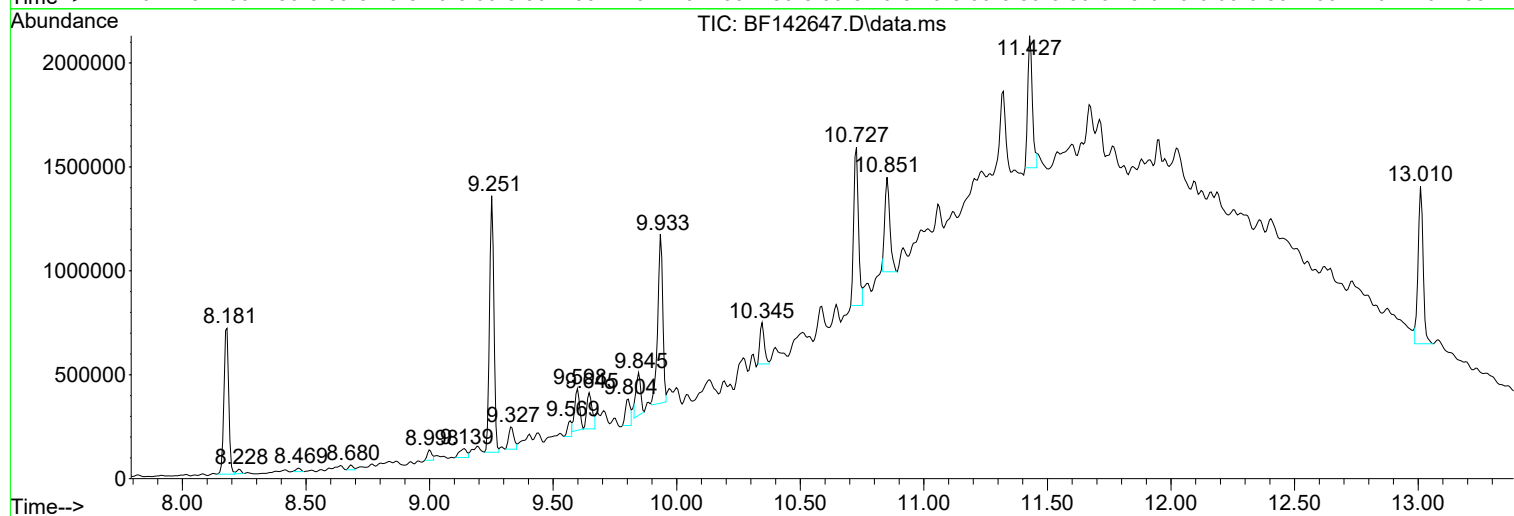
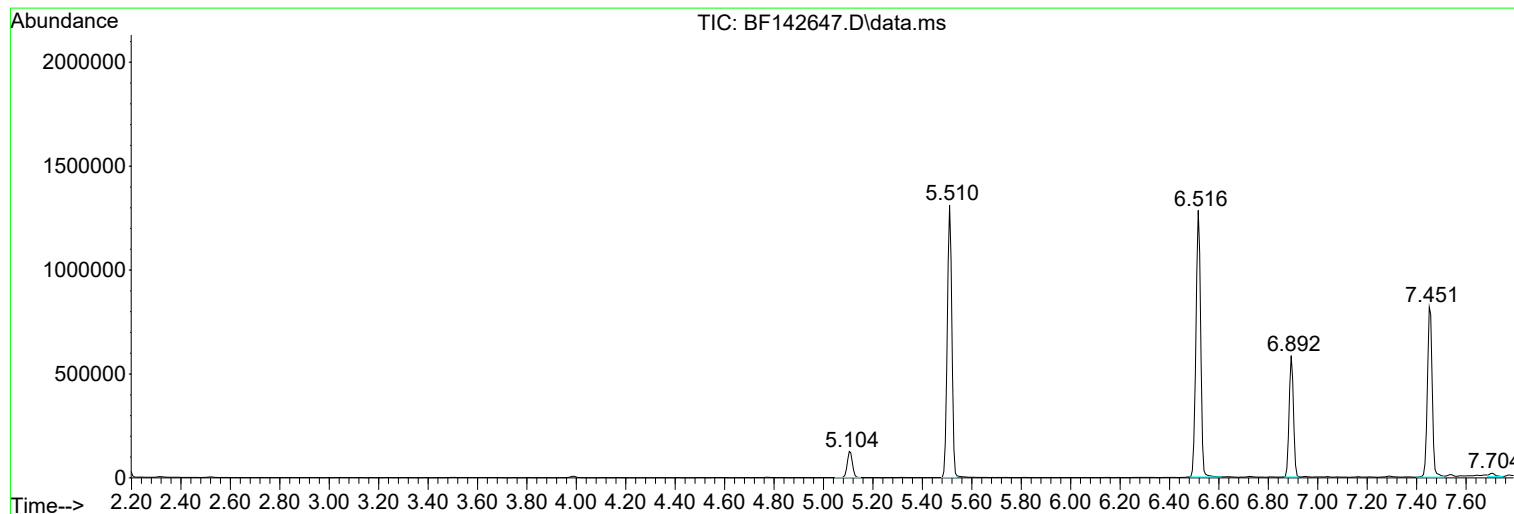
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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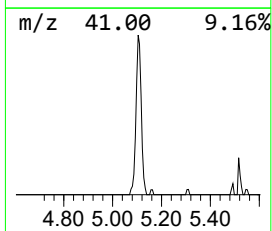
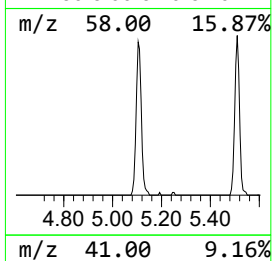
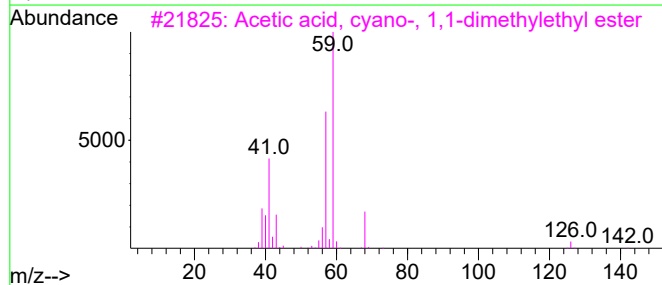
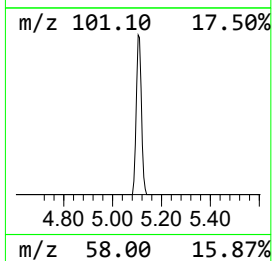
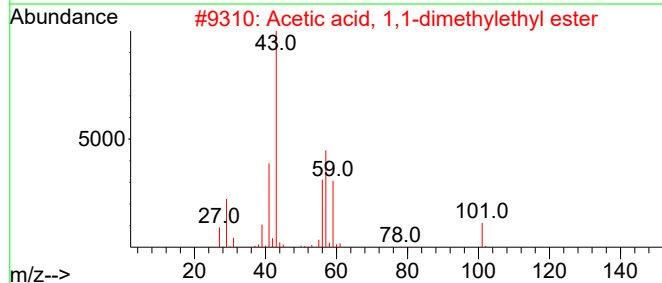
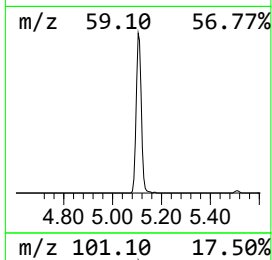
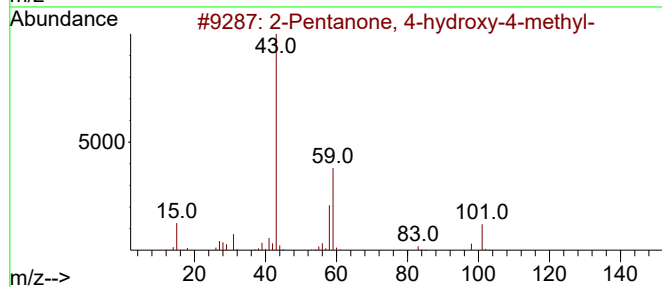
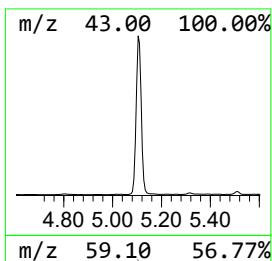
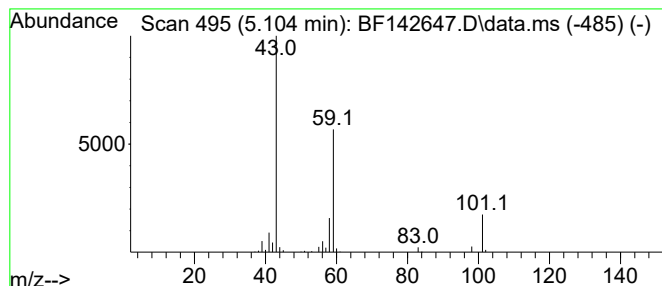
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.22 ng	185043	1,4-Dichlorobenzene-d4	6.892

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	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	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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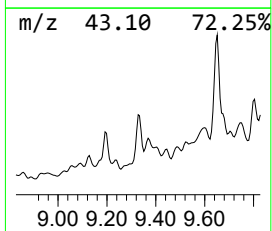
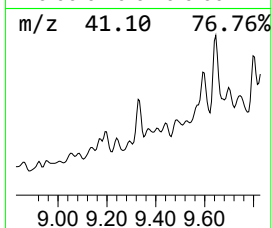
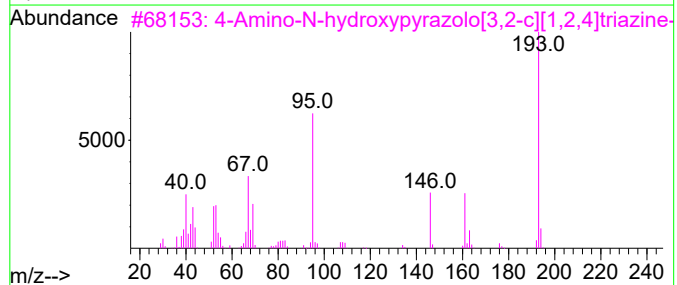
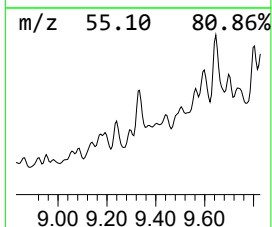
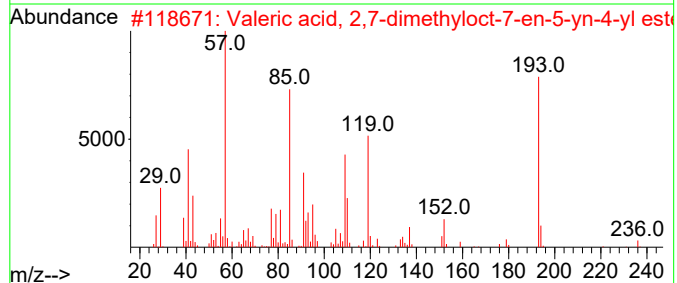
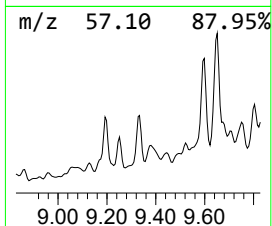
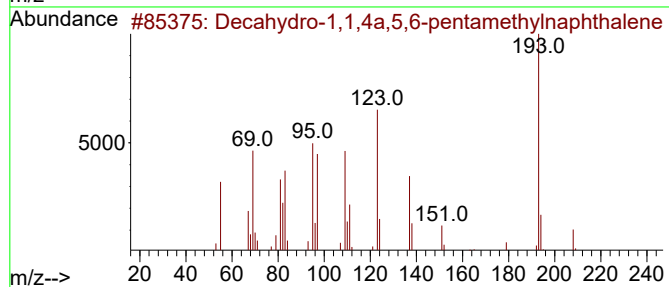
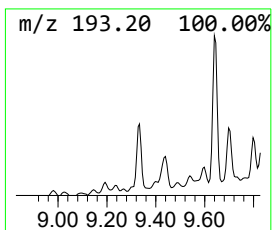
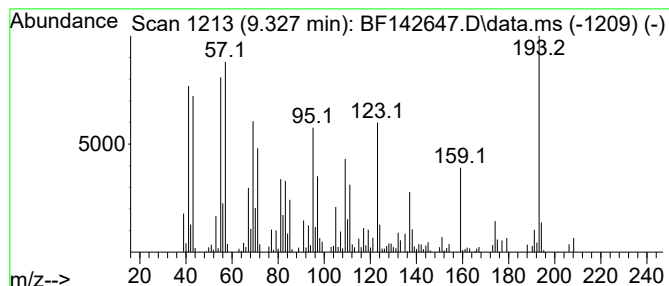
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown9.327 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.327	2.81 ng	162931	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2			Valeric acid, 2,7-dimethyloct-7-...	236	C15H24O2	1000292-48-9	35
3			4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	30
4			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	27
5			2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	22



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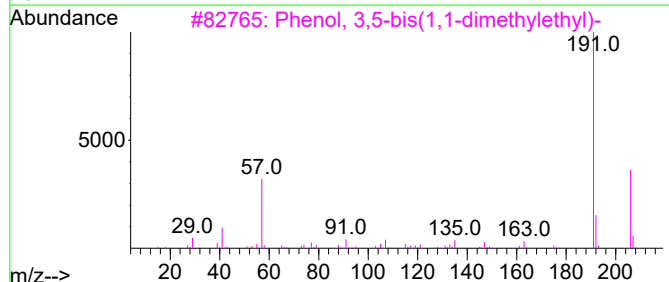
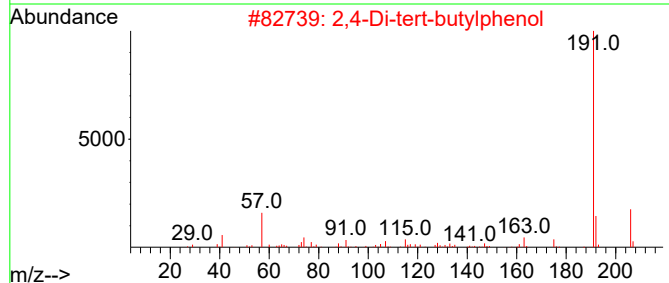
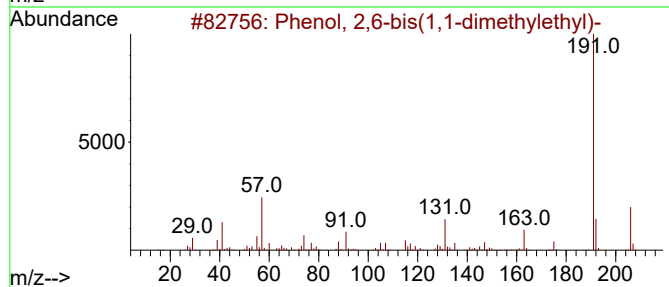
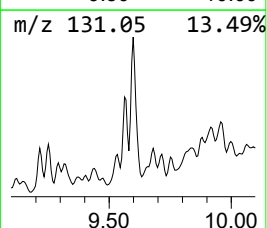
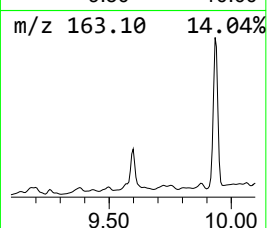
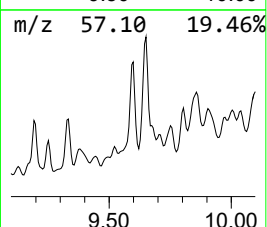
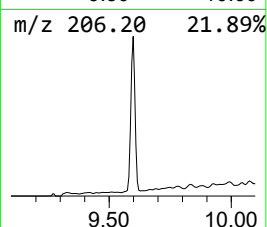
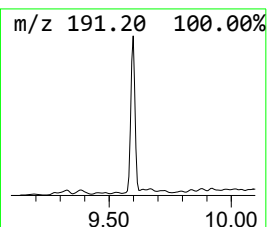
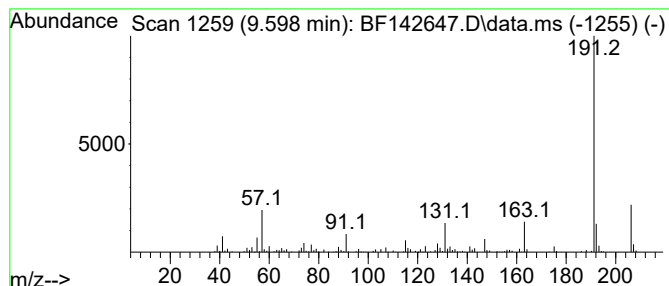
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Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.598	4.83 ng	280741	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
3			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	83
4			4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	72
5			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72



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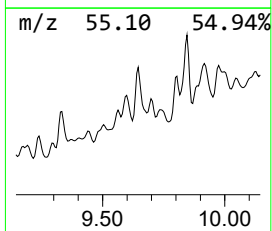
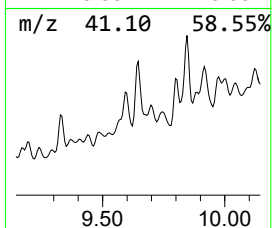
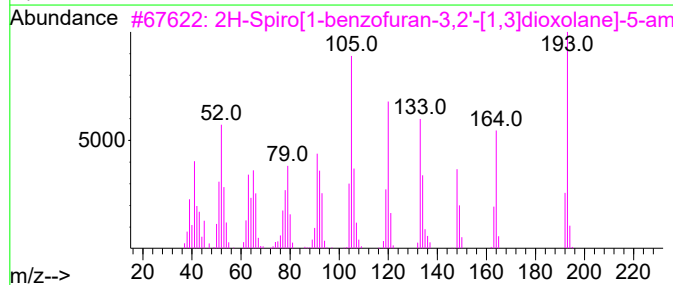
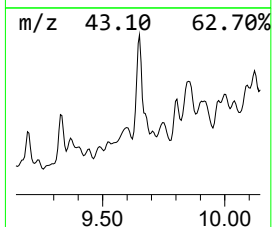
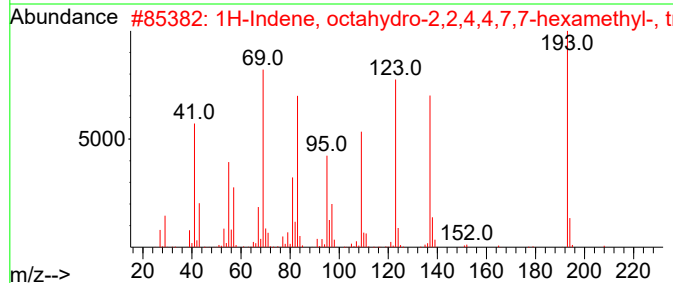
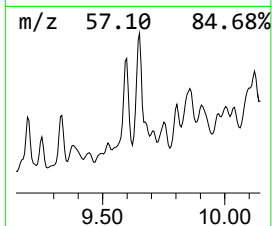
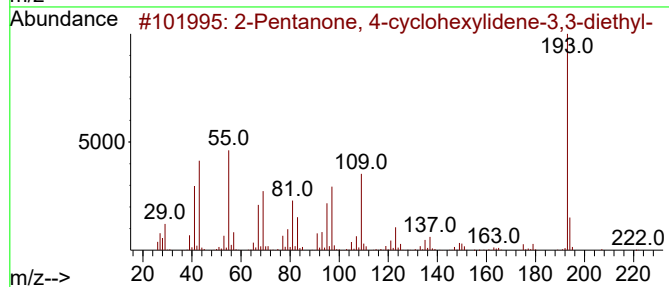
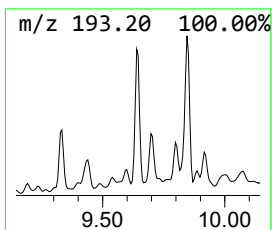
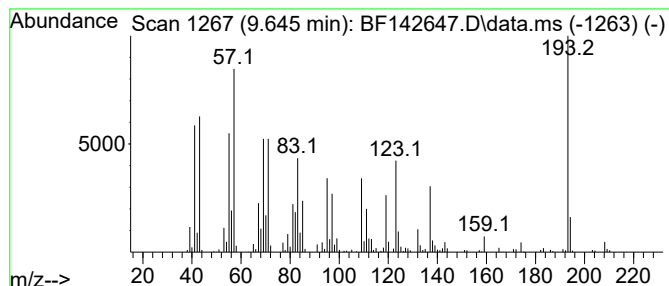
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Peak Number 4 unknown9.645 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.645	4.73 ng	274525	Acenaphthene-d10	9.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	43
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3	2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	30
4	Iminostilbene	193	C14H11N	000256-96-2	22
5	2-Amino-4-benzylthiomethyl-6-pip...	315	C16H21N5S	022362-19-2	22



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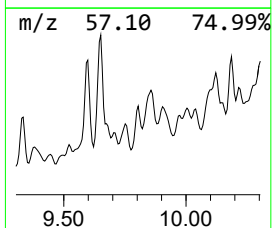
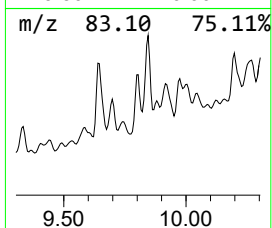
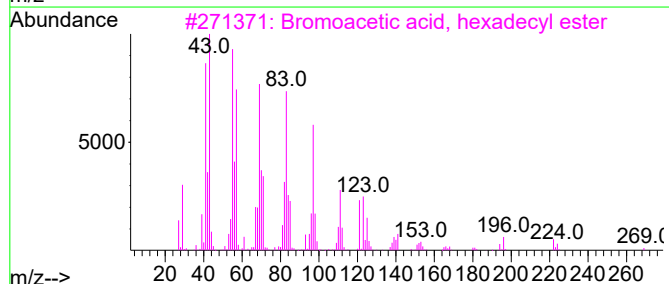
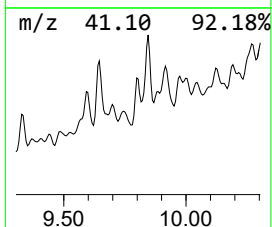
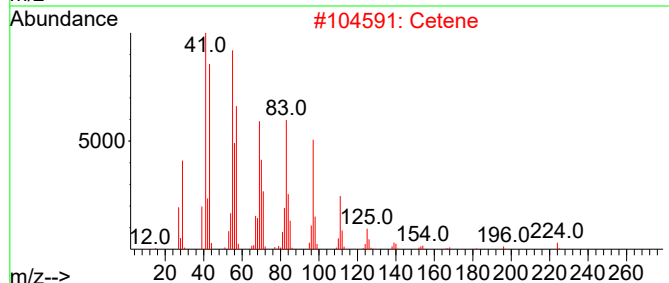
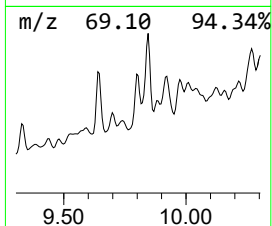
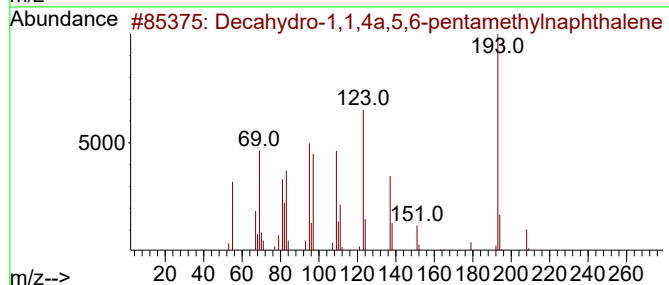
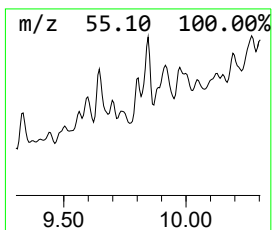
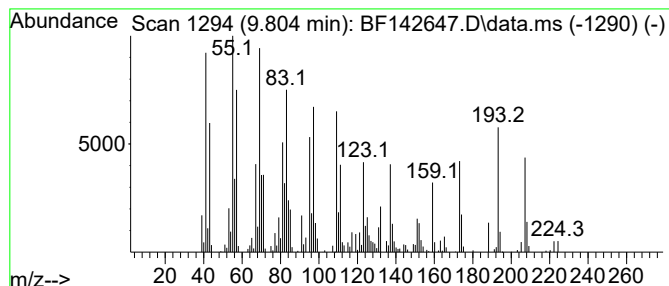
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Peak Number 5 unknown9.804 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	3.20 ng	185657	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	41
2			Cetene	224	C16H32	000629-73-2	38
3			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	30
4			1-Tricosene	322	C23H46	018835-32-0	30
5			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	30



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ClientSampleId :
RBR251425

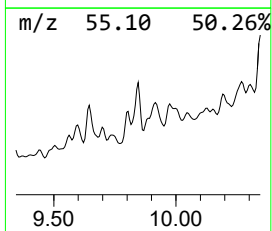
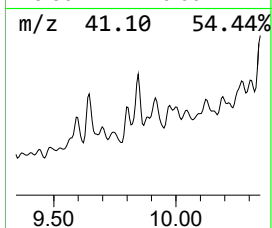
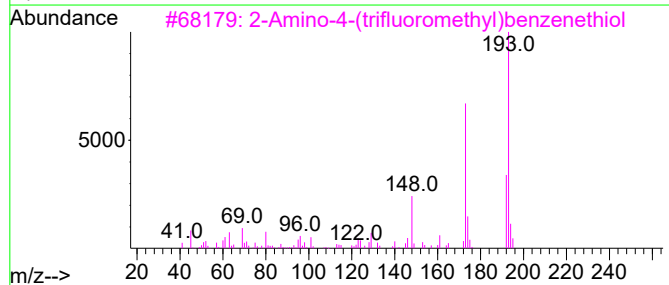
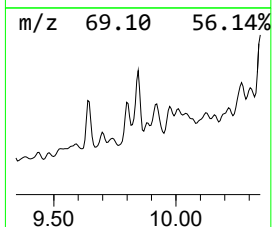
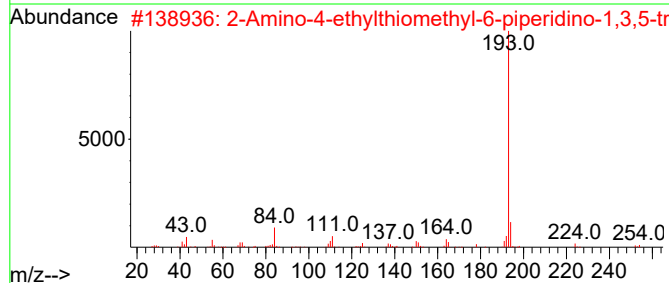
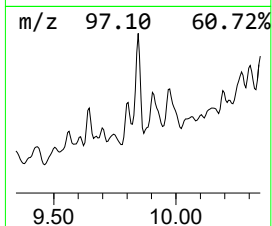
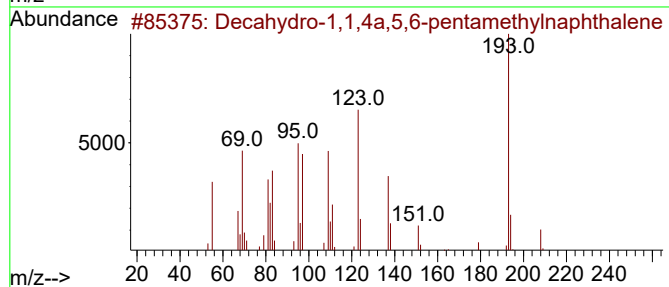
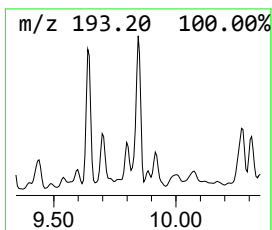
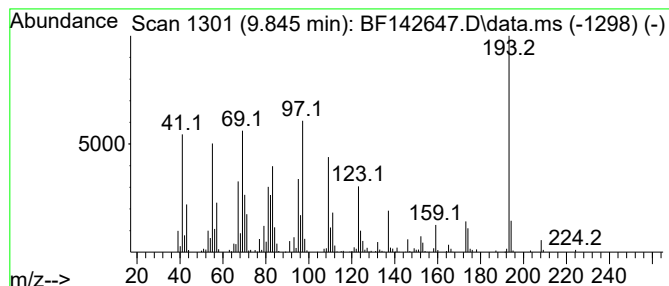
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.845 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.845	4.59 ng	266618	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2			2-Amino-4-ethylthiomethyl-6-pipe...	253	C11H19N5S	022362-22-7	22
3			2-Amino-4-(trifluoromethyl)benze...	193	C7H6F3NS	004274-38-8	22
4			Benzaldehyde, p-nitro-, dimethyl...	193	C9H11N3O2	010424-92-7	18
5			m-Nitrobenzaldehyde dimethylhydr...	193	C9H11N3O2	032787-76-1	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142647.D
Acq On : 06 Jun 2025 15:29
Operator : RC/JU
Sample : Q2214-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

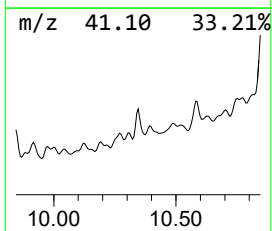
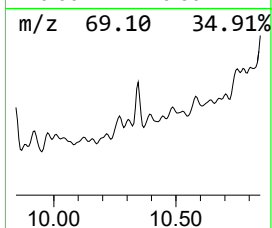
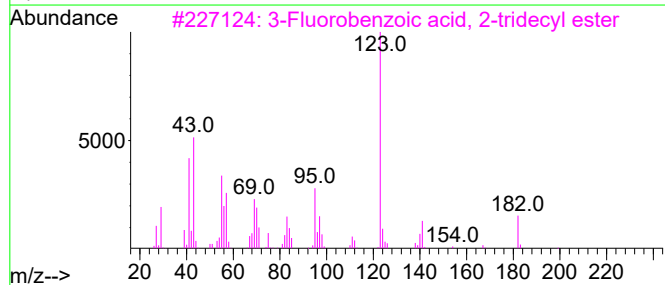
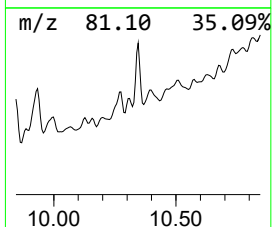
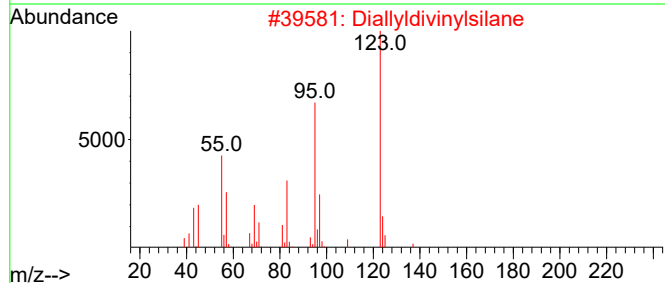
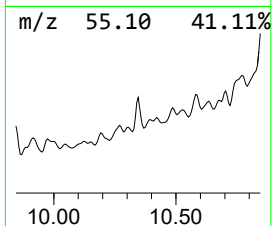
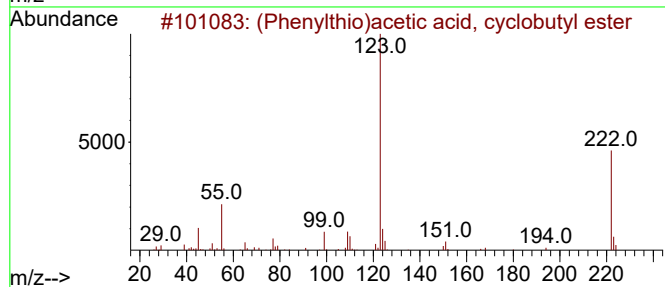
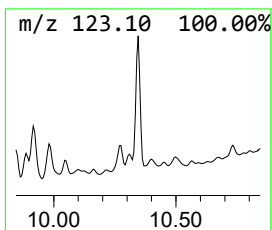
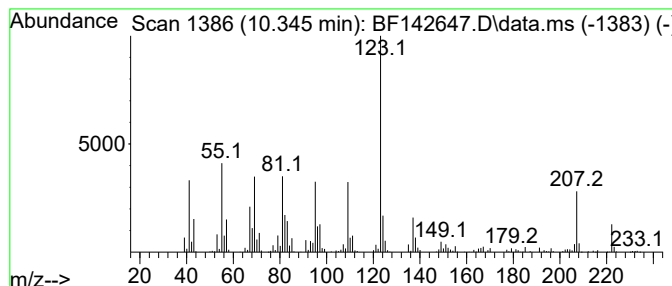
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ClientSampleId :
RBR251425

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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 (Phenylthio)acetic acid, cy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.345	4.34 ng	252260	Acenaphthene-d10		9.933	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1 (Phenylthio)acetic acid, cyclobu...		222	C12H14O2S	1010299-95-5	55
2	2 Diallyldivinylsilane		164	C10H16Si	119901-88-1	50
3	3 3-Fluorobenzoic acid, 2-tridecyl...		322	C20H31FO2	1000280-60-2	49
4	4 4-Fluorobenzoic acid, 6-ethyl-3-...		280	C17H25FO2	1000279-07-4	47
5	5 4-Fluorobenzoic acid, 3-pentadec...		350	C22H35FO2	1000280-68-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142647.D
Acq On : 06 Jun 2025 15:29
Operator : RC/JU
Sample : Q2214-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR251425

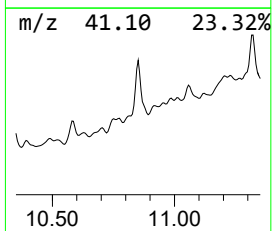
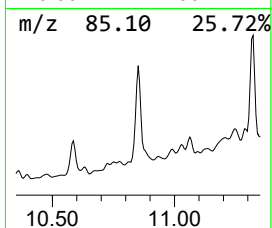
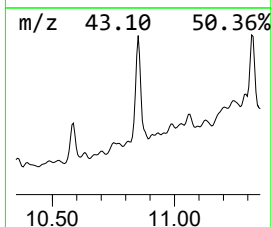
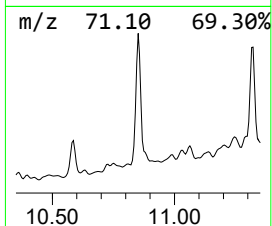
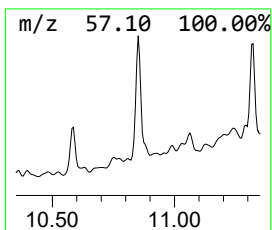
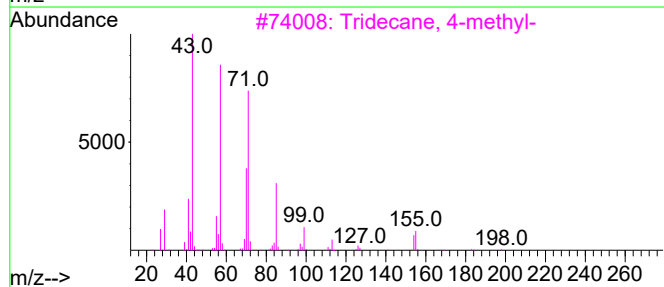
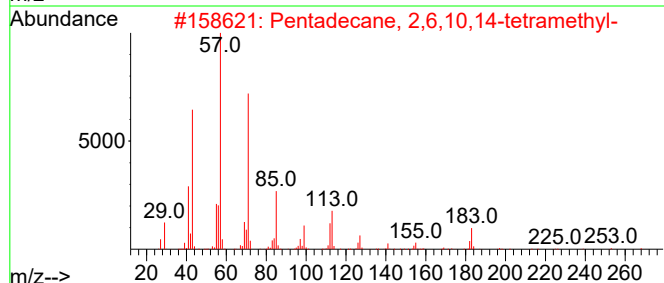
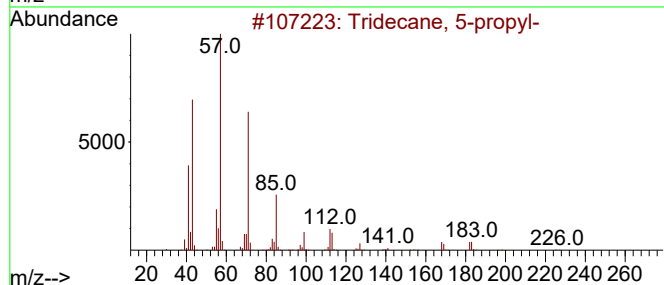
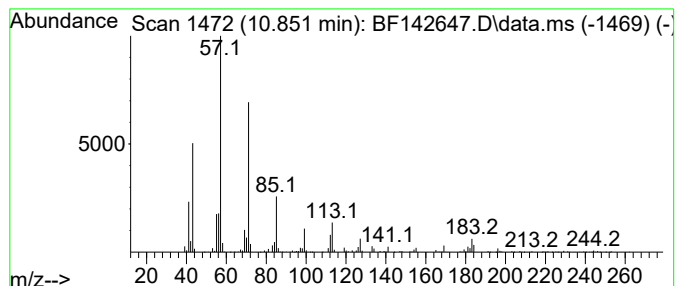
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 5-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	15.21 ng	634955	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
2			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	83
3			Tridecane, 4-methyl-	198	C14H30	026730-12-1	81
4			Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
5			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142647.D
Acq On : 06 Jun 2025 15:29
Operator : RC/JU
Sample : Q2214-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

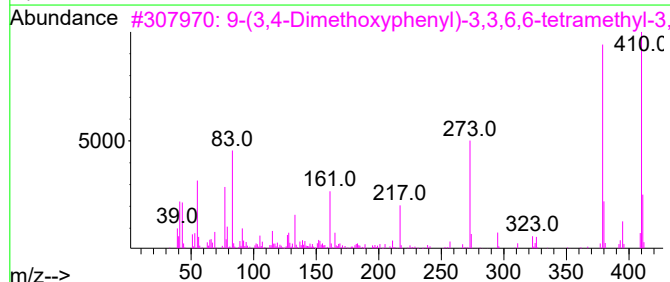
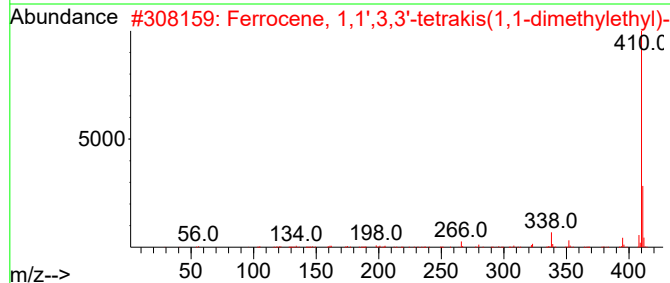
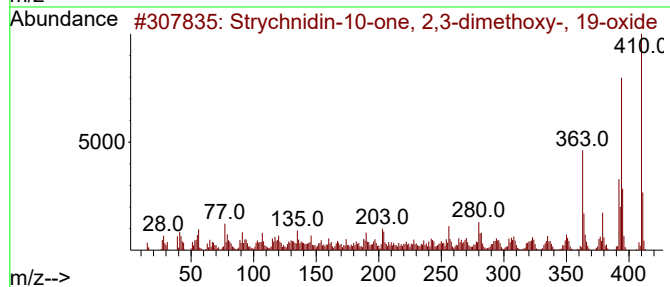
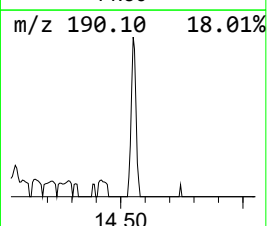
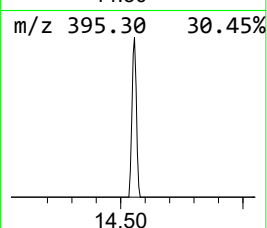
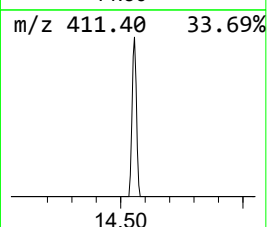
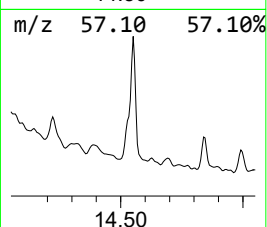
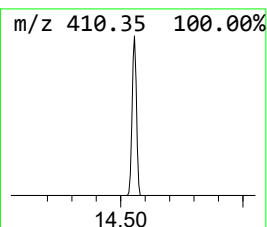
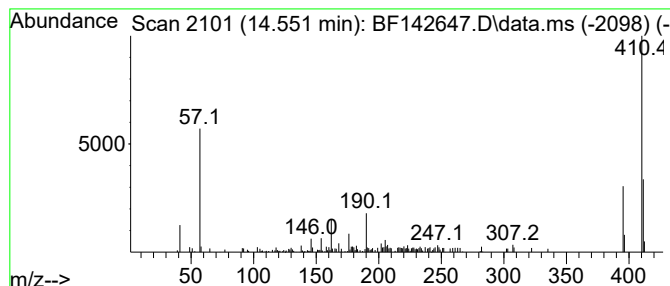
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Strychnidin-10-one, 2,3-dim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.551	3.26 ng	114131	Chrysene-d12		14.068	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Strychnidin-10-one, 2,3-dimethox...		410	C23H26N2O5	017301-81-4	72
2	Ferrocene, 1,1',3,3'-tetrakis(1,...		410	C26H42Fe	001317-17-5	53
3	9-(3,4-Dimethoxyphenyl)-3,3,6,6-...		410	C25H30O5	071827-94-6	45
4	3-Acetyl-1-(3,4-dimethoxyphenyl)...		410	C23H26N2O5	090140-65-1	45
5	Stigmasta-4,6,22-trien-3.beta.-ol		410	C29H46O	096737-58-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142647.D
Acq On : 06 Jun 2025 15:29
Operator : RC/JU
Sample : Q2214-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR251425

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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
2-Pentanone, 4-...	5.104	5.2	ng	185043	1	6.892	709632	20.0
unknown9.327	9.327	2.8	ng	162931	3	9.933	1161390	20.0
Phenol, 2,6-bis...	9.598	4.8	ng	280741	3	9.933	1161390	20.0
unknown9.645	9.645	4.7	ng	274525	3	9.933	1161390	20.0
unknown9.804	9.804	3.2	ng	185657	3	9.933	1161390	20.0
unknown9.845	9.845	4.6	ng	266618	3	9.933	1161390	20.0
(Phenylthio)ace...	10.345	4.3	ng	252260	3	9.933	1161390	20.0
Tridecane, 5-pr...	10.851	15.2	ng	634955	4	11.427	835047	20.0
Strychnidin-10-...	14.551	3.3	ng	114131	5	14.068	699172	20.0