

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
 Data File : BF131446.D
 Acq On : 29 Nov 2022 00:13
 Operator : CG\JU
 Sample : N5752-08 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-10D

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	17	22	29	rVB	248618	315763	32.33%	2.743%
2	2.328	36	41	54	rVB3	23319	40111	4.11%	0.348%
3	2.604	78	88	94	rVB	164988	242104	24.79%	2.103%
4	4.040	328	332	338	rBV	16463	19714	2.02%	0.171%
5	5.163	519	523	530	rVB	203064	199306	20.41%	1.732%
6	5.563	587	591	594	rBV	1097168	928772	95.10%	8.069%
7	6.569	758	762	766	rBV	1000795	890476	91.18%	7.736%
8	6.957	824	828	831	rBV	669704	592023	60.62%	5.143%
9	7.516	919	923	926	rBV	672278	539922	55.28%	4.691%
10	8.245	1043	1047	1050	rBV	884510	700790	71.75%	6.088%
11	9.322	1226	1230	1233	rBV	1290217	976654	100.00%	8.485%
12	9.398	1240	1243	1246	rBV2	38624	39849	4.08%	0.346%
13	9.533	1261	1266	1268	rBV6	13026	24597	2.52%	0.214%
14	9.710	1294	1296	1300	rBV3	51739	60125	6.16%	0.522%
15	9.875	1321	1324	1326	rBV	55696	58634	6.00%	0.509%
16	9.922	1328	1332	1335	rVB3	52109	60585	6.20%	0.526%
17	10.010	1341	1347	1350	rBV	773147	634432	64.96%	5.512%
18	10.322	1397	1400	1403	rBV2	40819	62161	6.36%	0.540%
19	10.416	1414	1416	1421	rVB3	45974	42122	4.31%	0.366%
20	10.804	1478	1482	1485	rBV	461799	442660	45.32%	3.846%
21	11.510	1599	1602	1604	rBV	800119	741543	75.93%	6.442%
22	11.533	1604	1606	1610	rVV	114955	167679	17.17%	1.457%
23	12.216	1721	1722	1725	rBV2	208553	195434	20.01%	1.698%
24	12.345	1742	1744	1746	rBV2	257852	305574	31.29%	2.655%
25	12.833	1823	1827	1831	rBV4	306825	553187	56.64%	4.806%
26	13.110	1871	1874	1880	rVB	800721	838982	85.90%	7.289%
27	14.174	2053	2055	2059	rVB	410024	389148	39.85%	3.381%
28	15.333	2251	2252	2256	rBV3	336183	412099	42.19%	3.580%
29	16.215	2400	2402	2405	rBV3	309095	484243	49.58%	4.207%
30	16.651	2475	2476	2479	rBV2	239059	182677	18.70%	1.587%
31	16.815	2502	2504	2510	rBV4	261484	369229	37.81%	3.208%

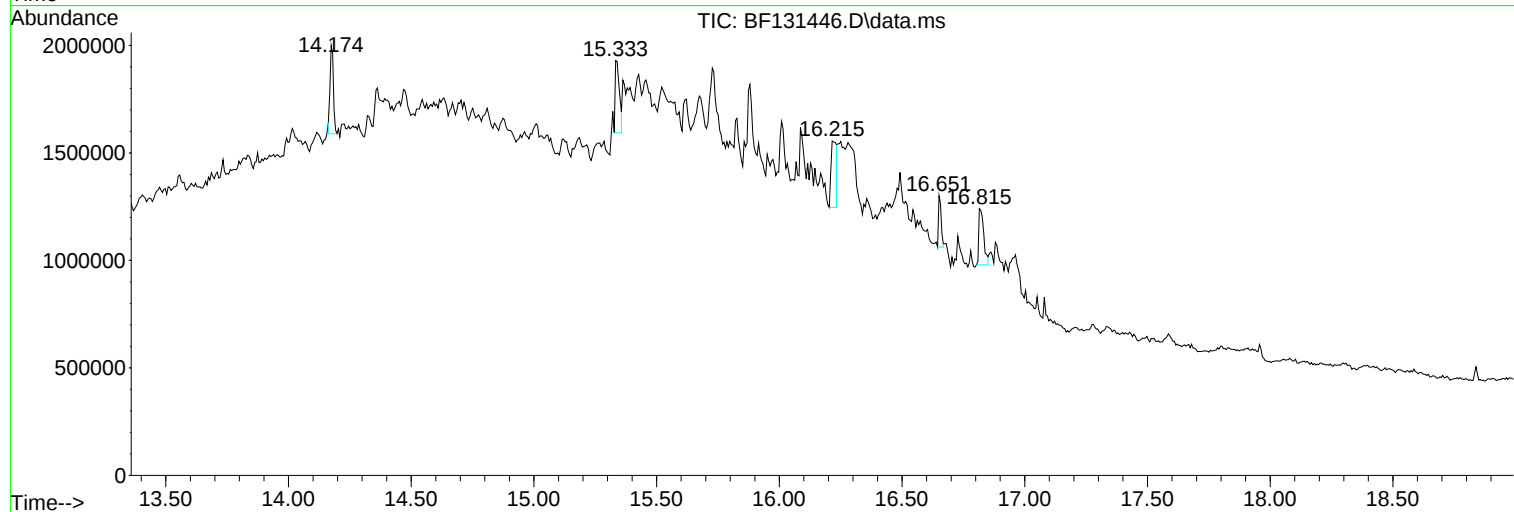
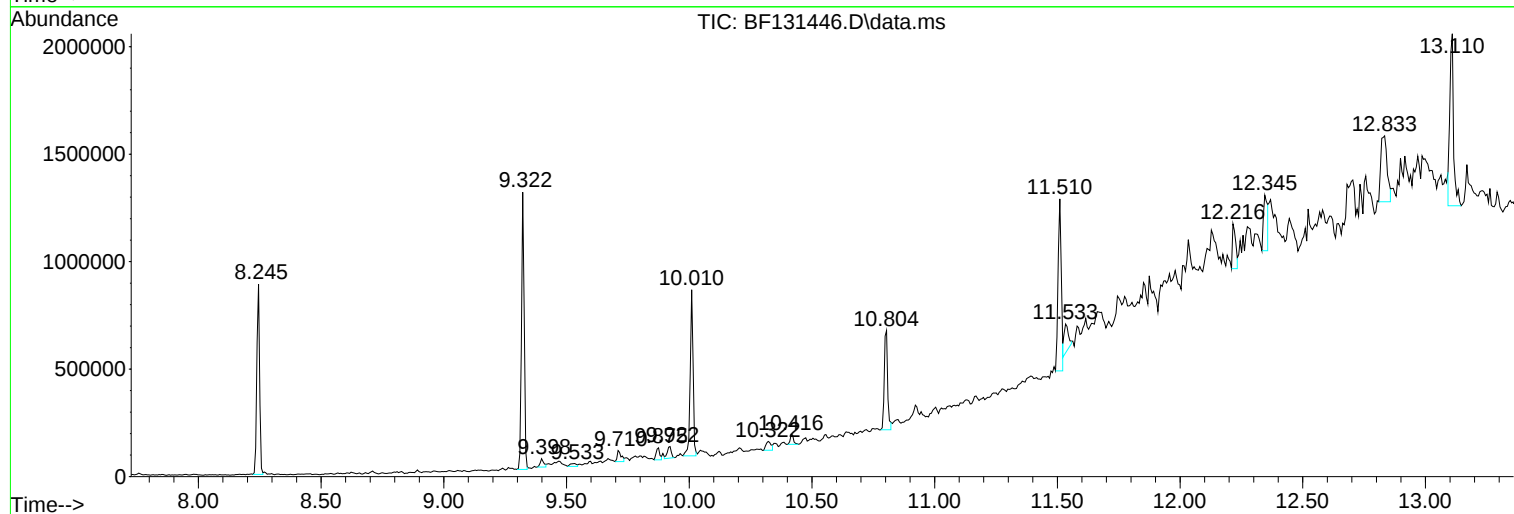
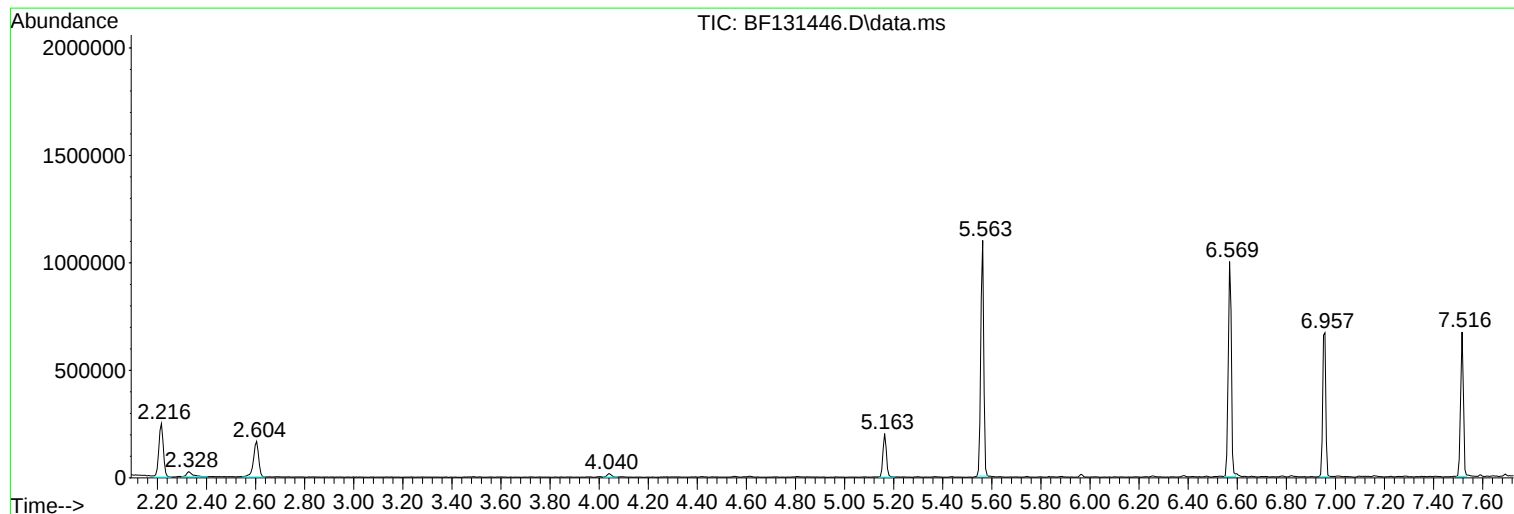
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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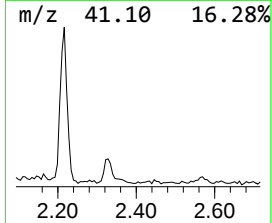
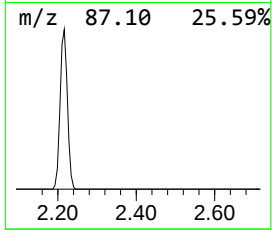
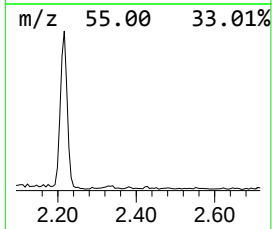
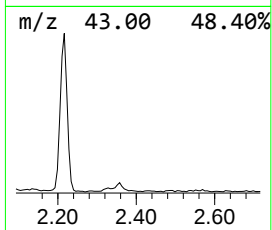
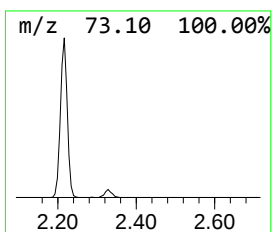
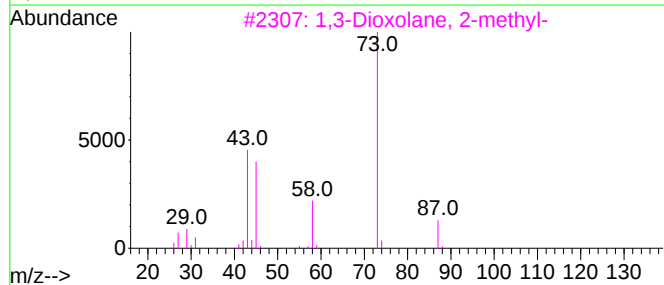
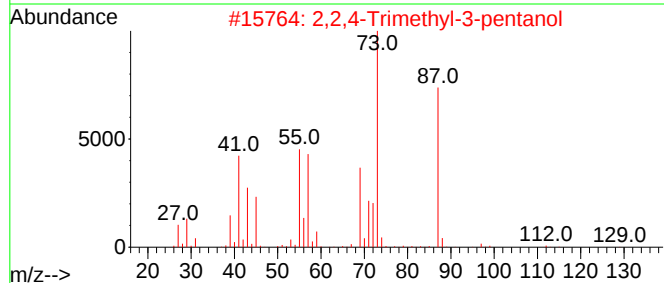
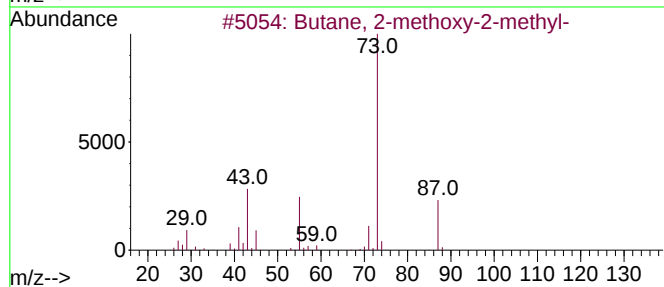
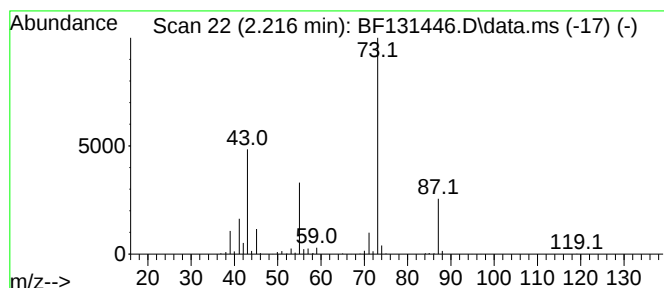
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	10.67 ng	315763	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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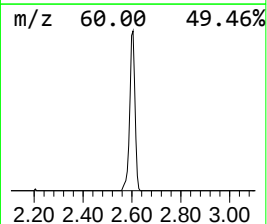
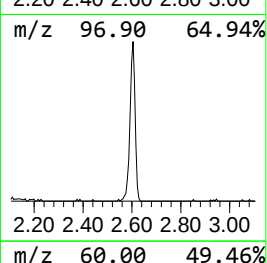
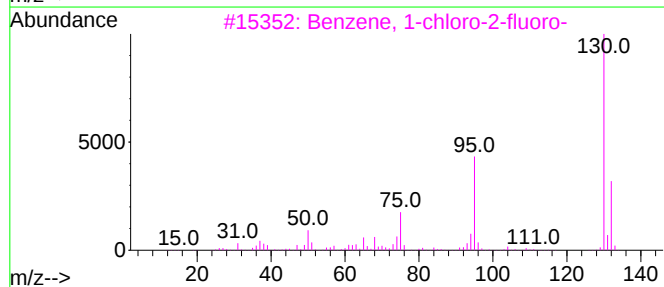
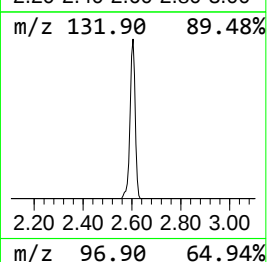
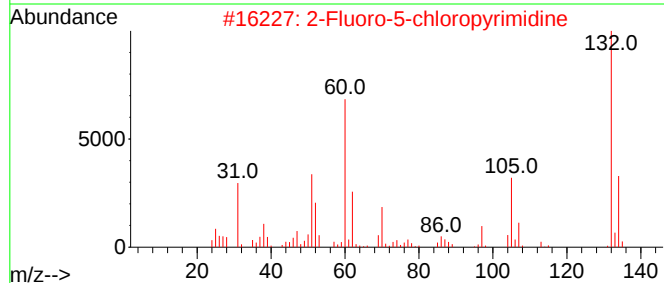
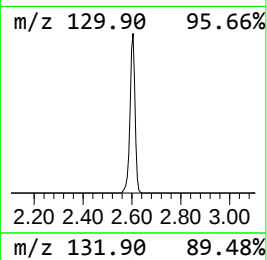
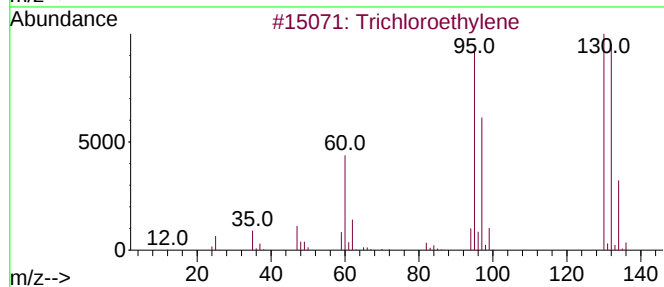
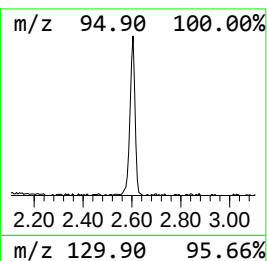
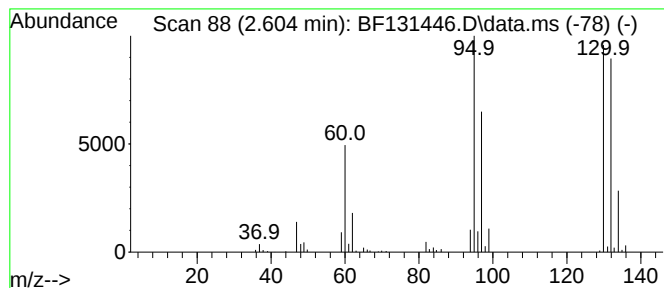
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Trichloroethylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.604	8.18 ng	242104	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroethylene	130	C2HCl3	000079-01-6	98
2			2-Fluoro-5-chloropyrimidine	132	C4H2ClFN2	062802-37-3	35
3			Benzene, 1-chloro-2-fluoro-	130	C6H4ClF	000348-51-6	25
4			Benzene, 1-chloro-4-fluoro-	130	C6H4ClF	000352-33-0	22
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	12



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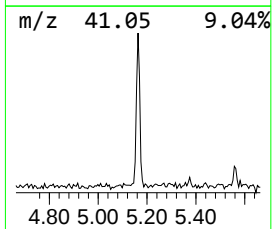
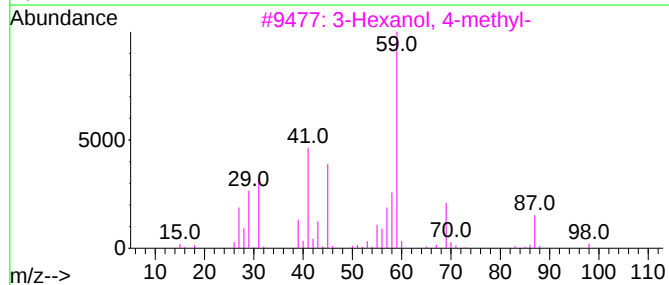
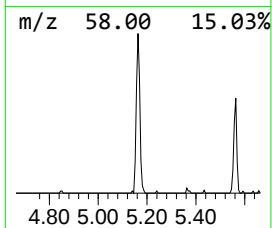
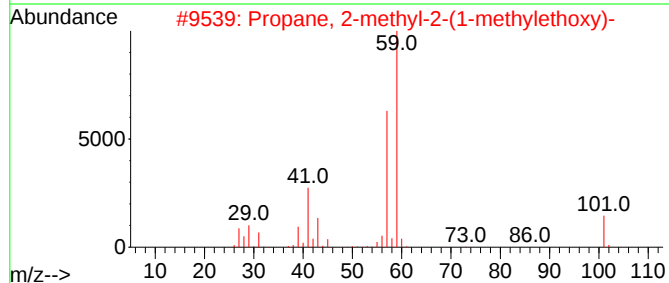
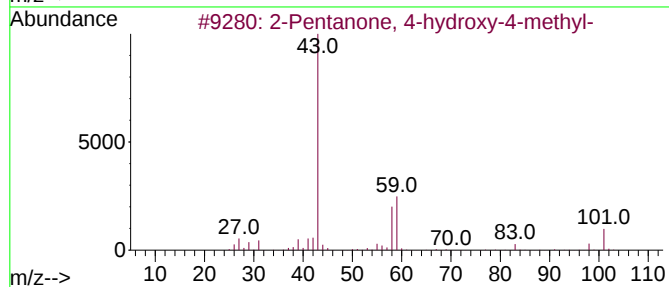
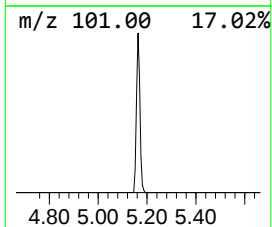
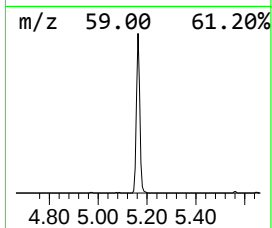
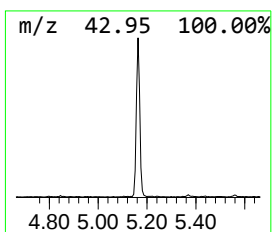
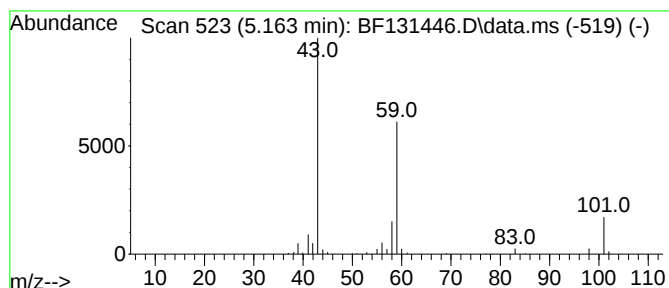
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	6.73 ng	199306	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			3-Octanol	130	C8H18O	000589-98-0	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33



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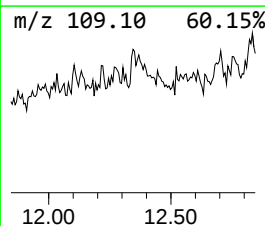
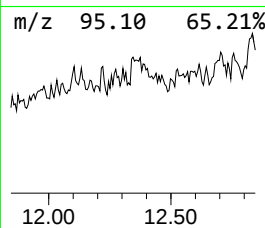
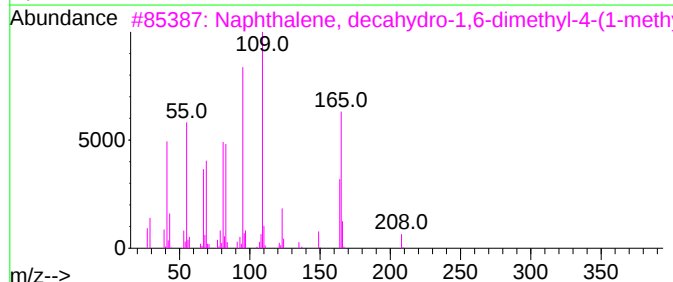
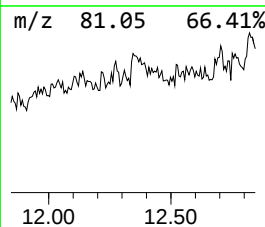
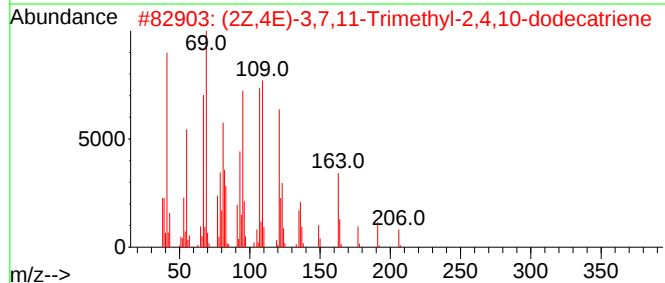
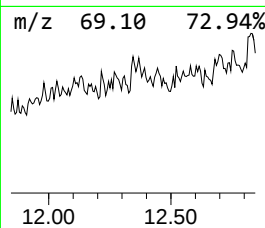
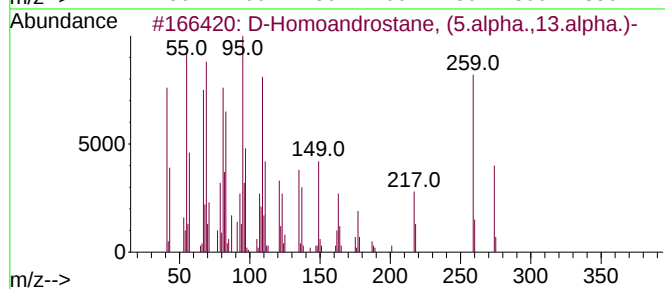
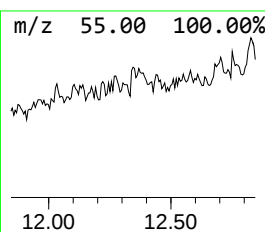
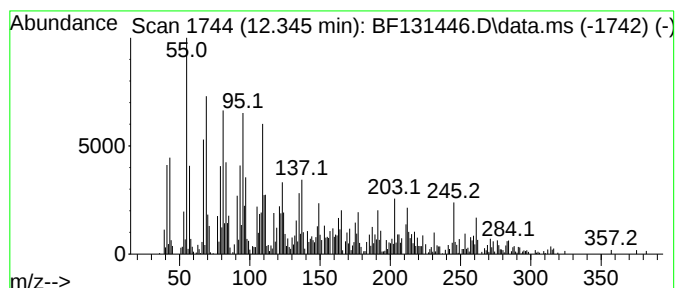
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Peak Number 5 D-Homoandrostande, (5.alpha.... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.345	8.24 ng	305574	Phenanthrene-d10	11.510	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Homoandrostande, (5.alpha.,13.a...	274	C20H34	054482-31-4	94
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	53
3	Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	46
4	Cyclohexene, 4-(4-ethylcyclohexy...	262	C19H34	301643-32-3	45
5	(1S,3E,7E,11E)-Cembra-3,7,11-triene	274	C20H34	1000432-97-5	41



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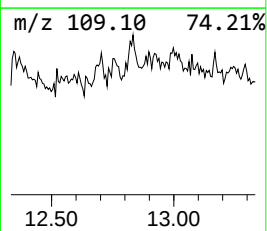
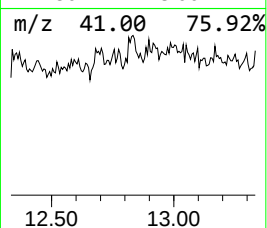
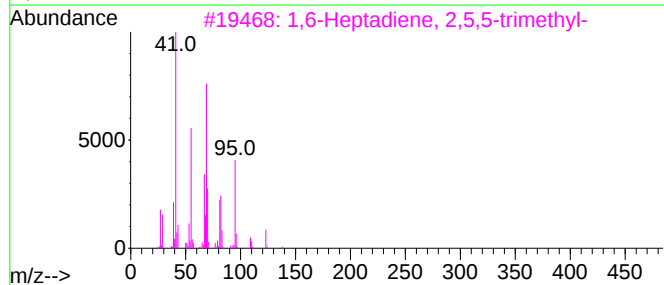
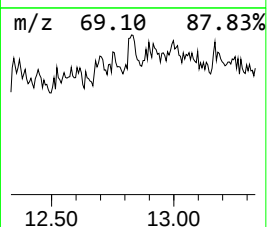
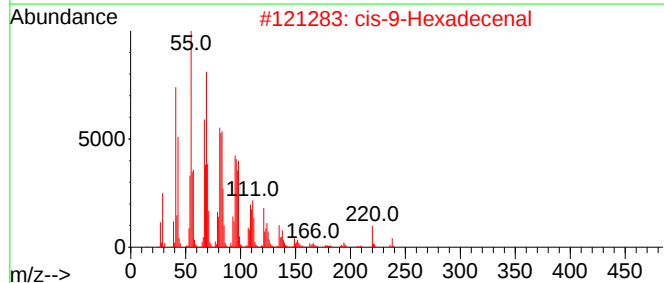
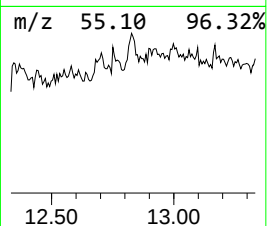
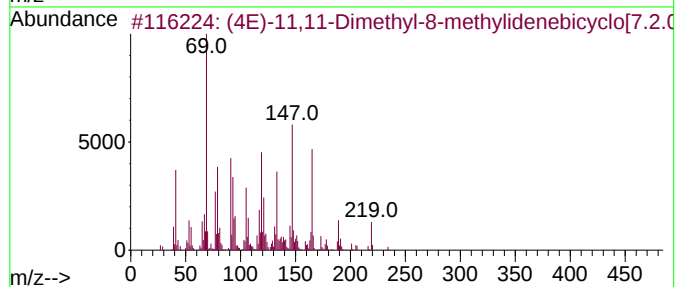
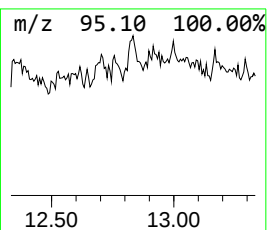
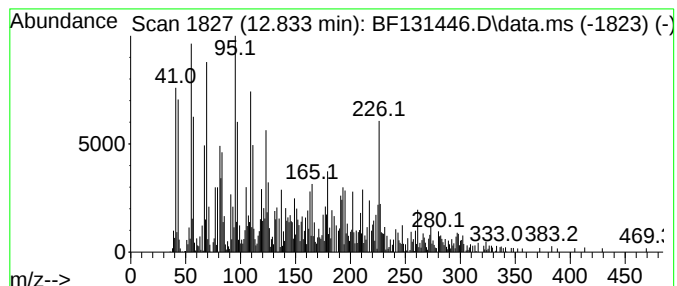
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Peak Number 6 unknown12.833 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.833	14.92 ng	553187	Phenanthrene-d10	11.510	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4E)-11,11-Dimethyl-8-methyliden...	234	C15H22O2	1000494-37-8	44
2	cis-9-Hexadecenal	238	C16H30O	056219-04-6	44
3	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	42
4	Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	38
5	9-Oxabicyclo[6.1.0]nonane, 1-met...	140	C9H16O	052954-47-9	35



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Misc :
ALS Vial : 19 Sample Multiplier: 1

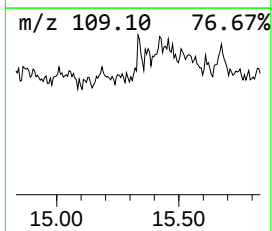
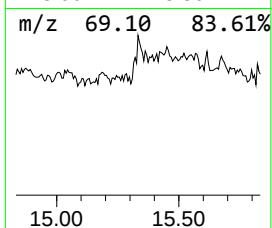
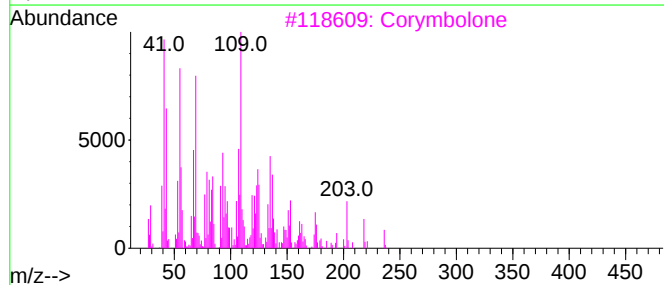
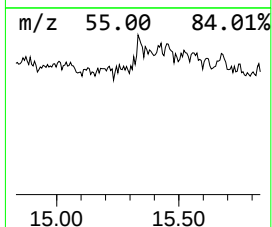
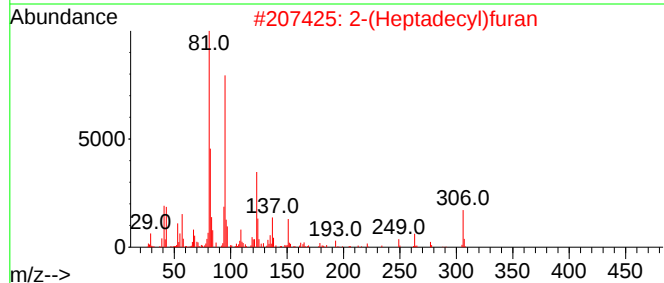
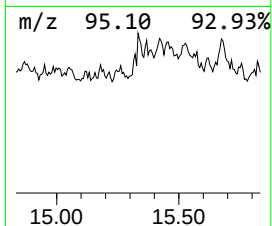
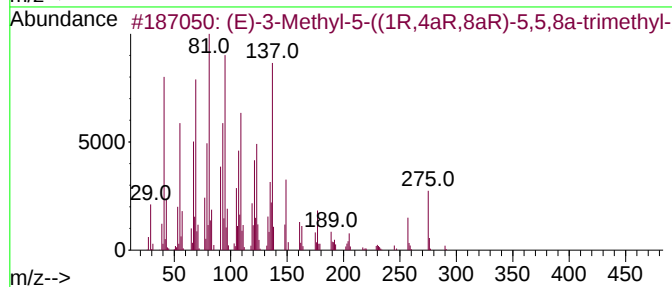
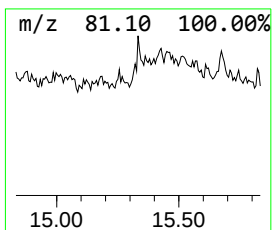
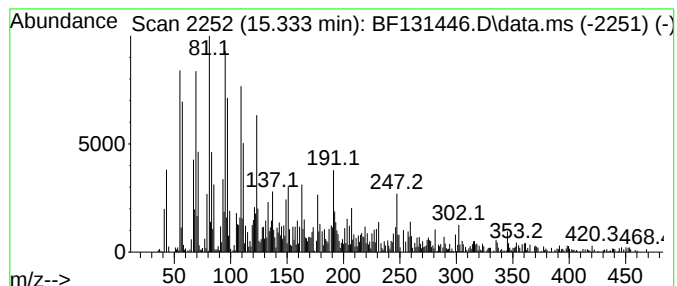
Instrument :
BNA_F
ClientSampleId :
B-10D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (E)-3-Methyl-5-((1R,4aR,8aR... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.333	20.00 ng	412099	Perylene-d12	15.733	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Methyl-5-((1R,4aR,8aR)-5,5...	290	C20H34O	021738-29-4	72
2	2-(Heptadecyl)furan	306	C21H38O	208329-97-9	52
3	Corymbolone	236	C15H24O2	097094-19-4	42
4	9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	41
5	3,5,9-Undecatrien-2-one, 6,10-di...	192	C13H20O	013927-47-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131446.D
Acq On : 29 Nov 2022 00:13
Operator : CG\JU
Sample : N5752-08 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

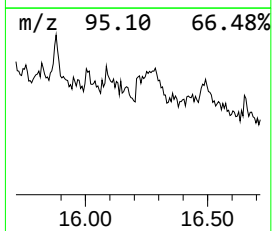
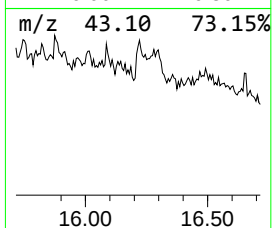
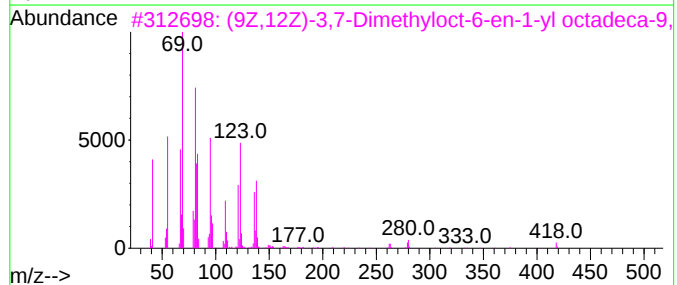
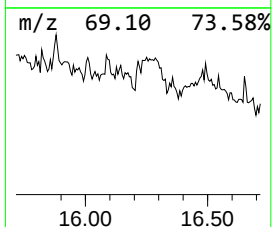
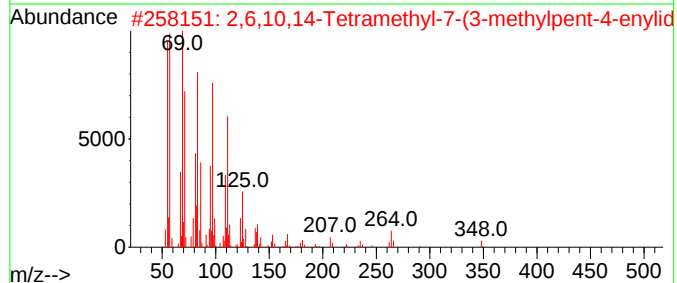
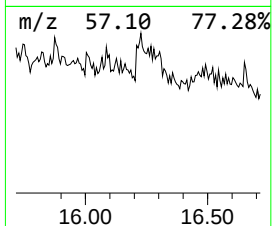
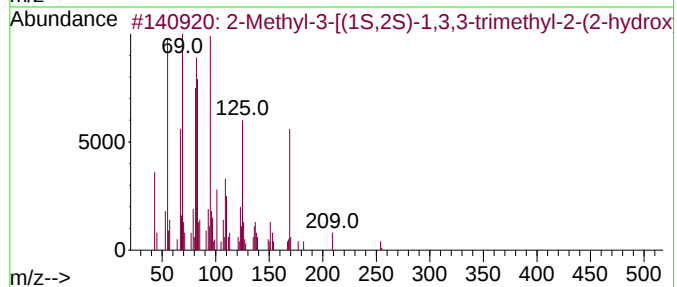
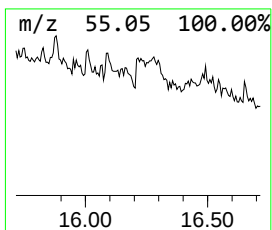
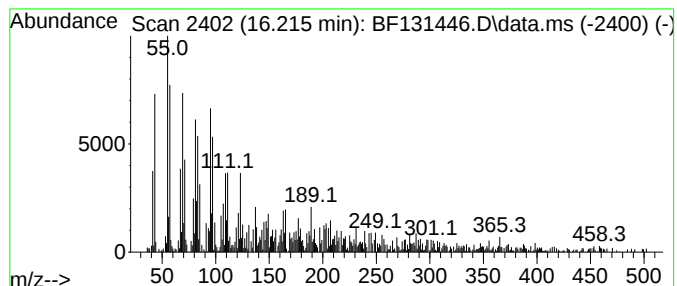
Instrument :
BNA_F
ClientSampleId :
B-10D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Methyl-3-[(1S,2S)-1,3,3-t... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	23.50 ng	484243	Perylene-d12	15.733
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1	2-Methyl-3-[(1S,2S)-1,3,3-trimet...	254 C16H30O2	1000111-77-6	62
2	2,6,10,14-Tetramethyl-7-(3-methy...	348 C25H48	1000370-41-6	55
3	(9Z,12Z)-3,7-Dimethyloct-6-en-1-...	418 C28H50O2	1000412-98-8	51
4	Bicyclo[3.1.1]heptan-3-one, 2-(b...	192 C13H20O	1010163-96-1	50
5	Benzonitrile, 2-fluoro-4-(4'-pro...	327 C22H30FN	093743-04-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131446.D
Acq On : 29 Nov 2022 00:13
Operator : CG\JU
Sample : N5752-08 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-10D

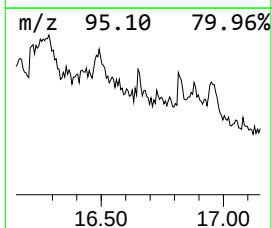
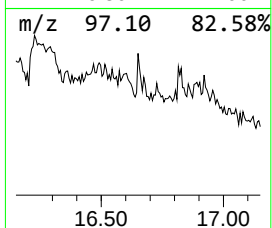
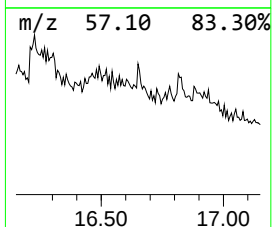
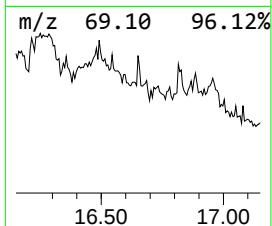
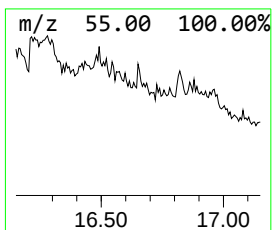
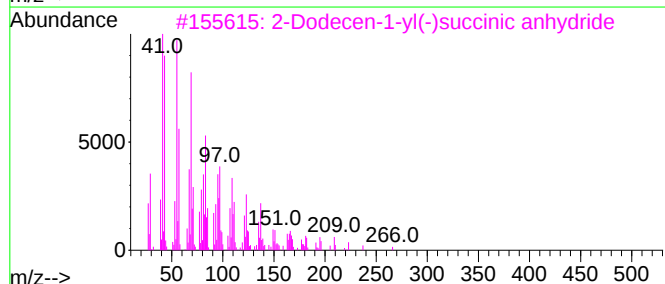
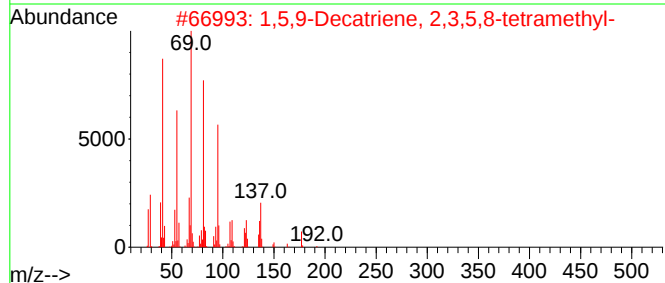
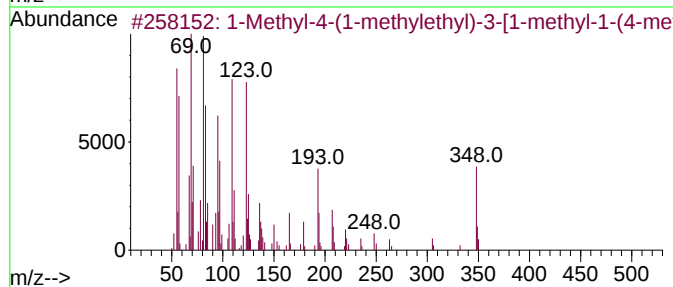
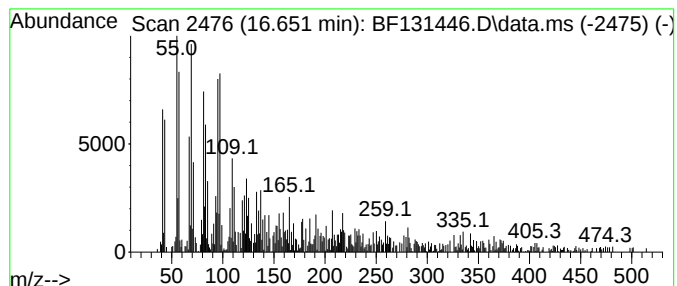
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Methyl-4-(1-methylethyl)-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.651	8.87 ng	182677	Perylene-d12	15.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-4-(1-methylethyl)-3-[1-...	348	C25H48	1000370-41-4	60		
2	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	58		
3	2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	46		
4	2,6,10,14-Tetramethyl-7-(3-methy...	348	C25H48	1000370-41-6	45		
5	Marrubiin	332	C20H28O4	000465-92-9	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131446.D
Acq On : 29 Nov 2022 00:13
Operator : CG\JU
Sample : N5752-08 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

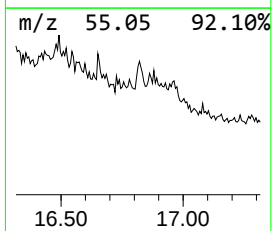
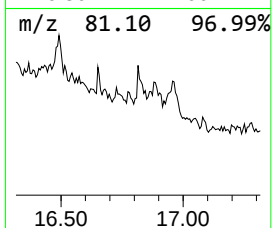
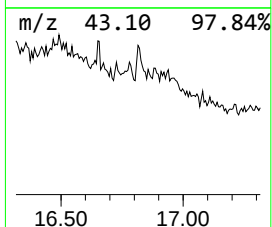
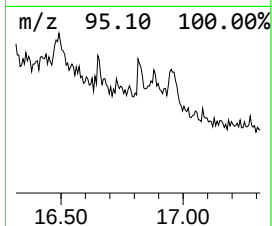
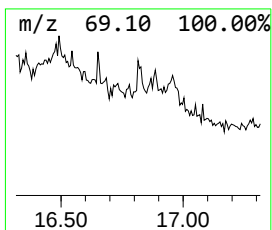
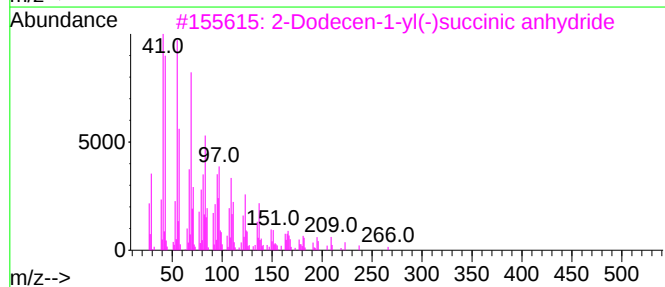
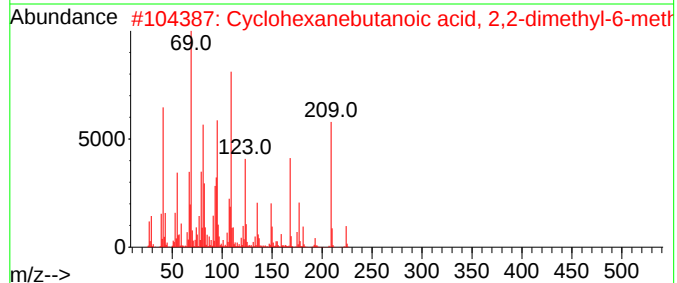
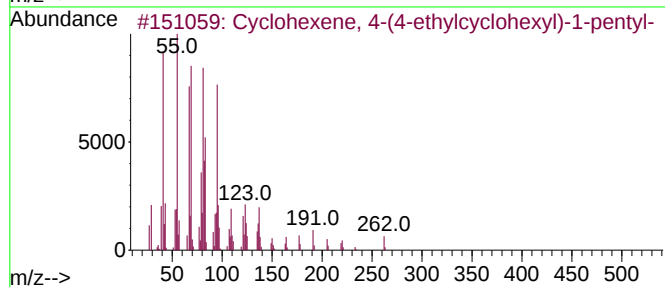
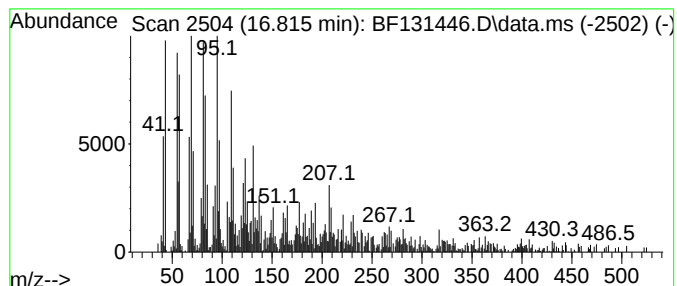
Instrument :
BNA_F
ClientSampleId :
B-10D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexene, 4-(4-ethylcycl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.815	17.92 ng	369229	Perylene-d12	15.733	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 4-(4-ethylcyclohexy...	262	C19H34	301643-32-3	70
2	Cyclohexanebutanoic acid, 2,2-di...	224	C14H24O2	095452-15-6	66
3	2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	64
4	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	64
5	Humulane-1,6-dien-3-ol	222	C15H26O	1000140-23-1	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131446.D
Acq On : 29 Nov 2022 00:13
Operator : CG\JU
Sample : N5752-08 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-10D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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
Butane, 2-metho...	2.216	10.7	ng	315763	1	6.957	592023	20.0
Trichloroethylene	2.604	8.2	ng	242104	1	6.957	592023	20.0
2-Pentanone, 4-...	5.163	6.7	ng	199306	1	6.957	592023	20.0
11,13-Dimethyl-...	12.216	5.3	ng	195434	4	11.510	741543	20.0
D-Homoandrostan...	12.345	8.2	ng	305574	4	11.510	741543	20.0
unknown12.833	12.833	14.9	ng	553187	4	11.510	741543	20.0
(E)-3-Methyl-5-...	15.333	20.0	ng	412099	6	15.733	412099	20.0
2-Methyl-3-[(1S...	16.215	23.5	ng	484243	6	15.733	412099	20.0
1-Methyl-4-(1-m...	16.651	8.9	ng	182677	6	15.733	412099	20.0
Cyclohexene, 4-...	16.815	17.9	ng	369229	6	15.733	412099	20.0