

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
 Data File : BF125865.D
 Acq On : 15 Oct 2021 16:26
 Operator : JU/CG
 Sample : M4242-21
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T2-COMP-(1-4)

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-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125865.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	1577774	1895588	42.92%	6.063%
2	5.063	501	506	514	rVB	85004	111248	2.52%	0.356%
3	5.457	565	573	576	rBV	3718616	3588702	81.26%	11.478%
4	6.463	738	744	747	rBV	3529221	3597278	81.45%	11.506%
5	6.833	803	807	810	rBV	1321849	1031647	23.36%	3.300%
6	7.392	894	902	905	rBV	2488250	2390957	54.14%	7.647%
7	8.016	1004	1008	1012	rBV	246375	222443	5.04%	0.711%
8	8.116	1020	1025	1028	rBV	1511436	1401769	31.74%	4.483%
9	9.186	1202	1207	1211	rBV	4684249	4416314	100.00%	14.125%
10	9.575	1271	1273	1277	rBV2	79895	80046	1.81%	0.256%
11	9.733	1294	1300	1303	rBV3	139652	207971	4.71%	0.665%
12	9.780	1306	1308	1310	rVB	151931	109411	2.48%	0.350%
13	9.816	1310	1314	1316	rBV4	70352	86261	1.95%	0.276%
14	9.863	1316	1322	1326	rBV	1637732	1582060	35.82%	5.060%
15	9.904	1326	1329	1334	rBV3	137268	210010	4.76%	0.672%
16	9.980	1340	1342	1345	rBV2	78430	78242	1.77%	0.250%
17	10.204	1378	1380	1383	rVB	292930	254258	5.76%	0.813%
18	10.239	1383	1386	1389	rBV3	327145	407606	9.23%	1.304%
19	10.274	1390	1392	1395	rBV2	333648	291242	6.59%	0.932%
20	10.327	1398	1401	1406	rVV3	360876	516906	11.70%	1.653%
21	10.651	1453	1456	1459	rBV	1699917	1855543	42.02%	5.935%
22	11.357	1573	1576	1578	rBV	1084130	1010665	22.88%	3.233%
23	12.945	1843	1846	1849	rVB	2580155	2288785	51.83%	7.321%
24	13.992	2021	2024	2027	rVB	1123073	1008290	22.83%	3.225%
25	15.015	2195	2198	2208	rVB	319688	573981	13.00%	1.836%
26	15.374	2257	2259	2262	rVB	146178	131077	2.97%	0.419%
27	15.439	2266	2270	2274	rBV	898867	1086519	24.60%	3.475%
28	16.139	2386	2389	2407	rVB2	178473	438994	9.94%	1.404%
29	16.574	2459	2463	2469	rVB	135066	224971	5.09%	0.720%
30	16.874	2510	2514	2521	rVB2	91352	166621	3.77%	0.533%

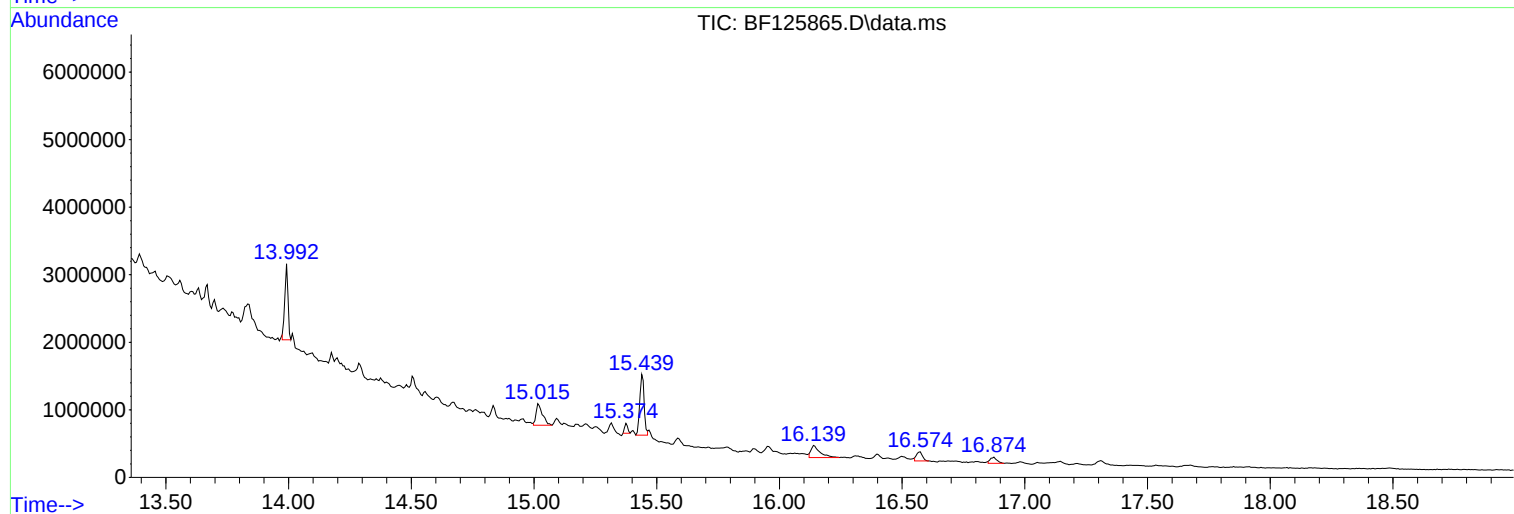
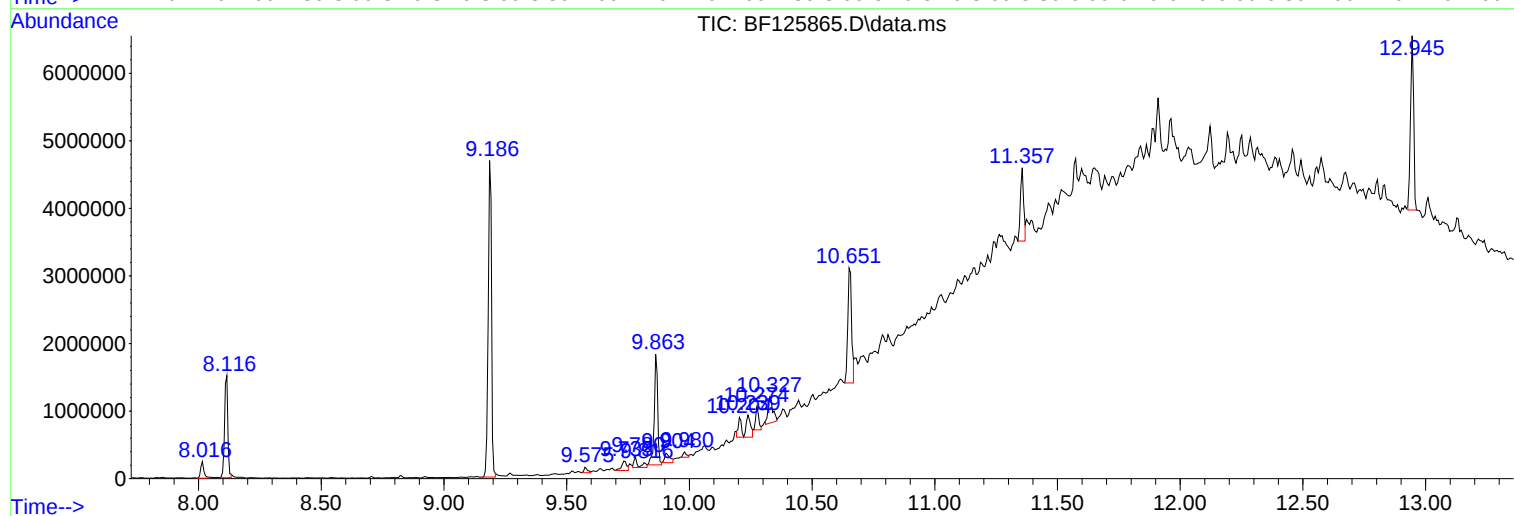
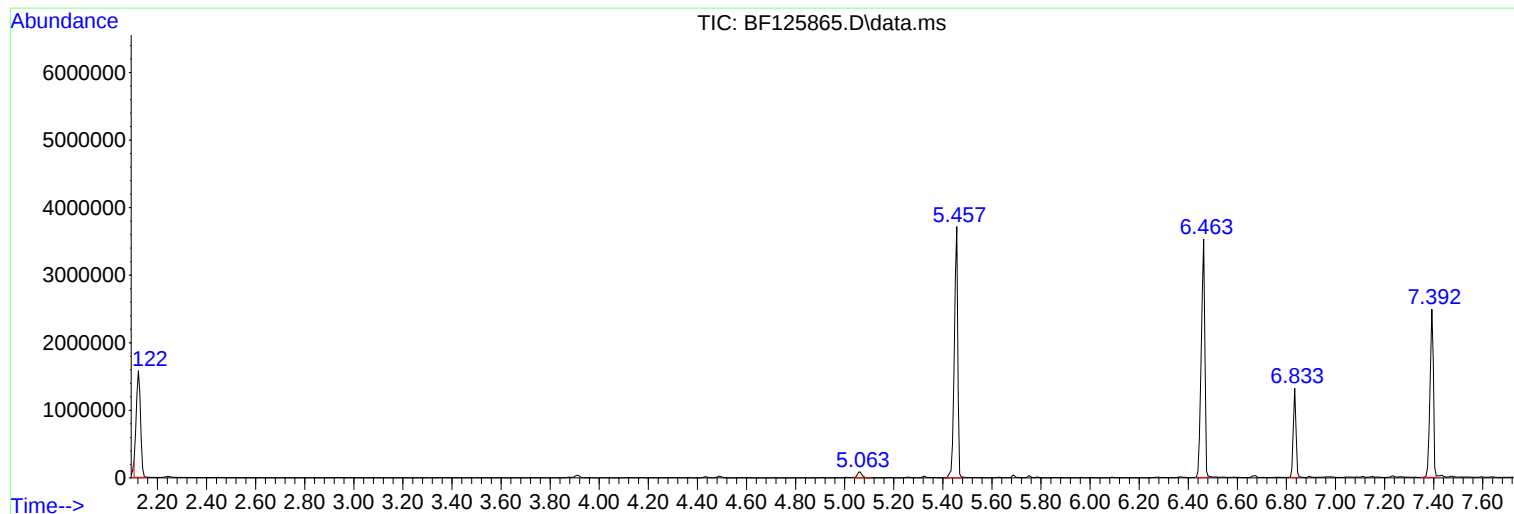
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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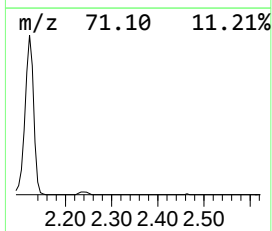
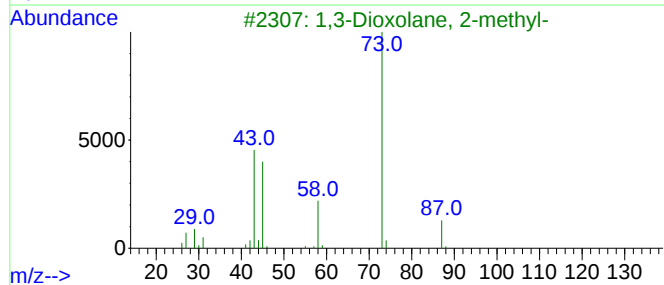
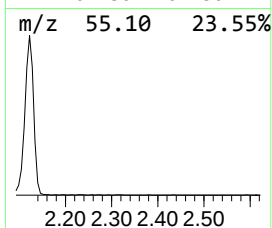
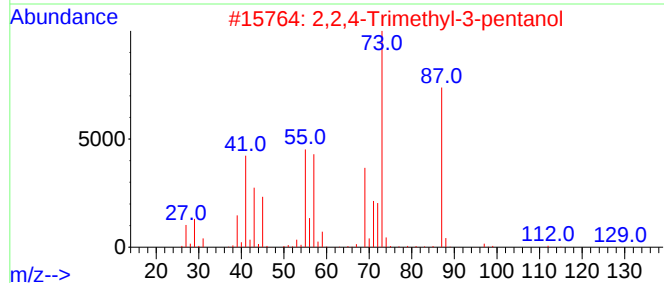
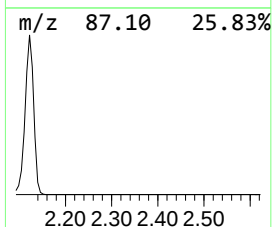
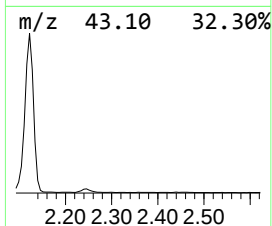
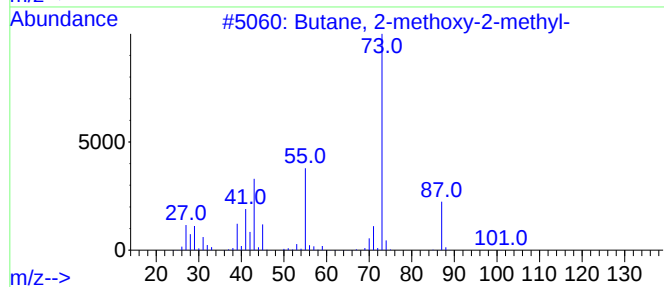
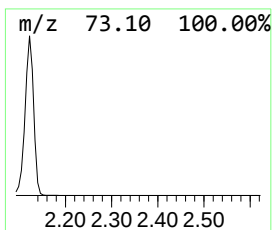
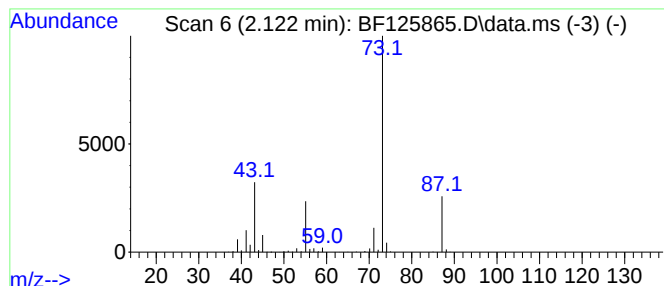
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	36.75 ng	1895590	1,4-Dichlorobenzene-d4	6.833

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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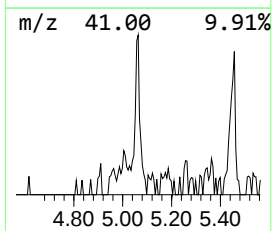
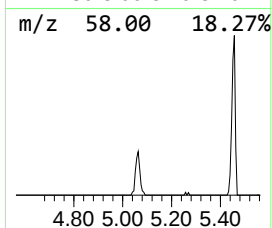
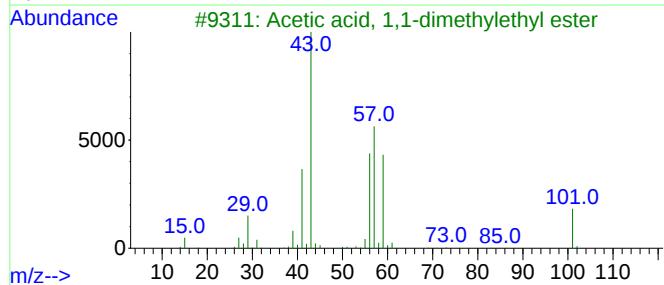
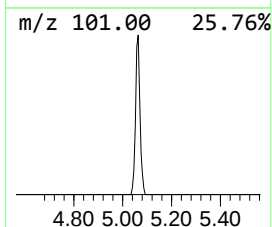
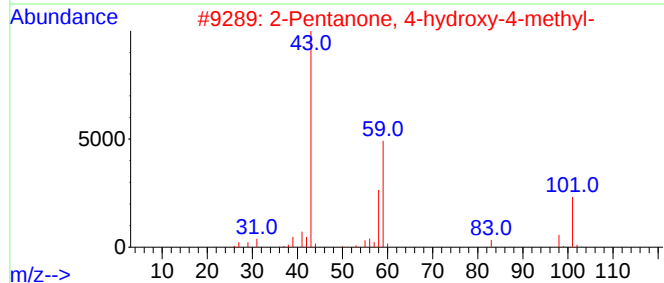
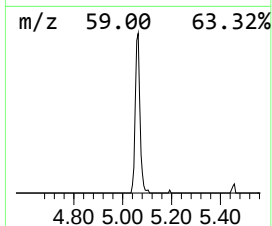
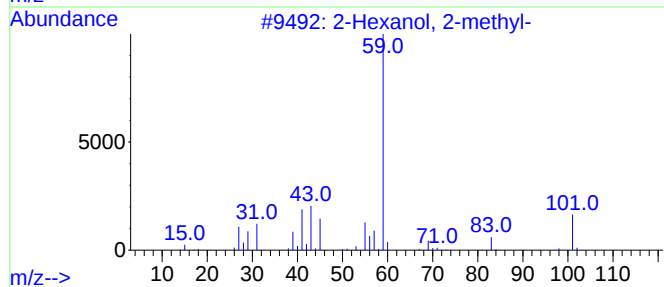
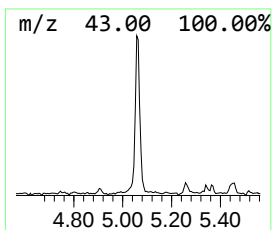
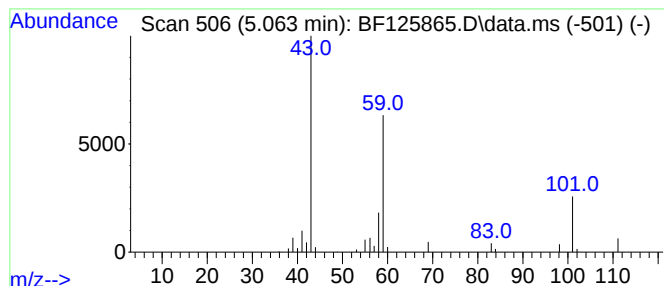
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.063 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	2.16 ng	111248	1,4-Dichlorobenzene-d4	6.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	37
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	32
5			Methyl 16-methoxyheptadecanoate	314	C19H38O3	1000110-18-2	17



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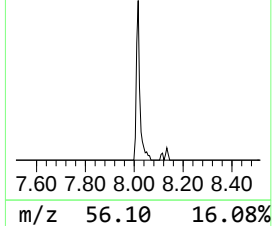
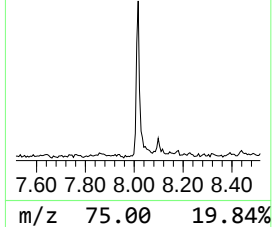
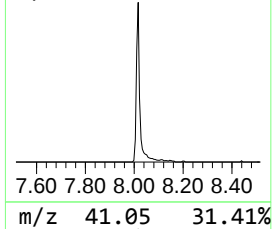
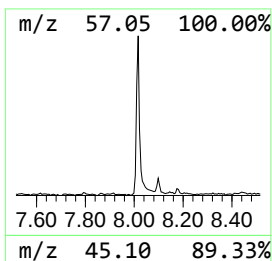
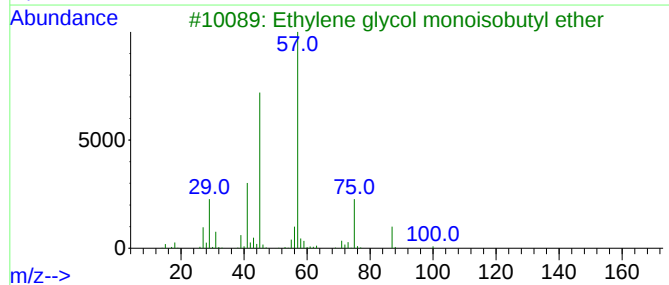
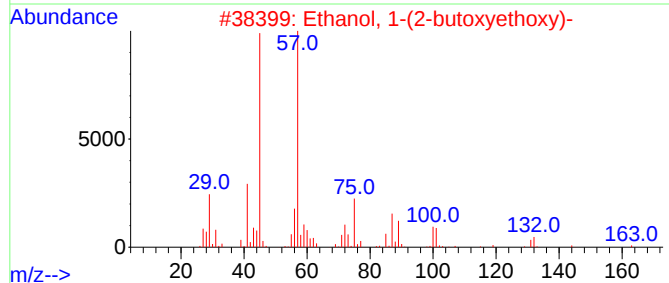
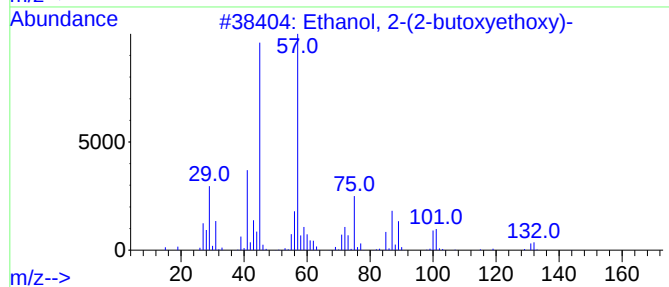
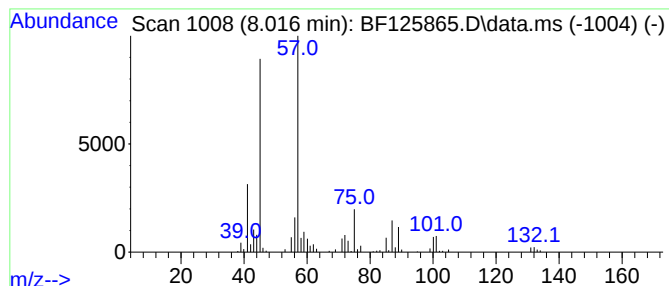
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	3.17 ng	222443	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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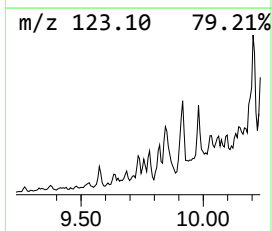
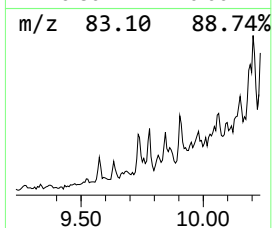
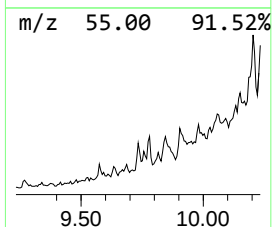
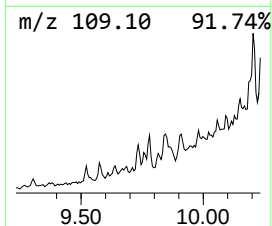
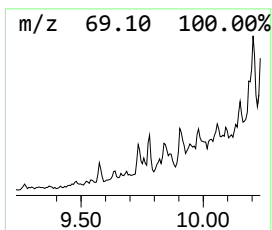
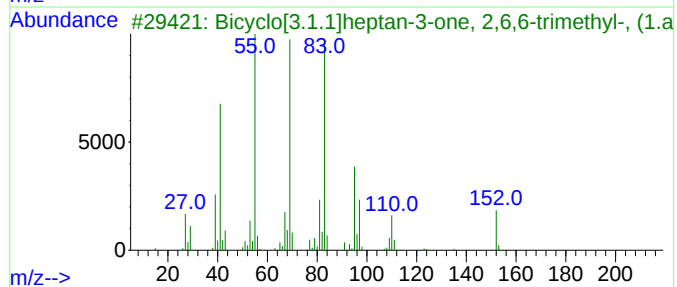
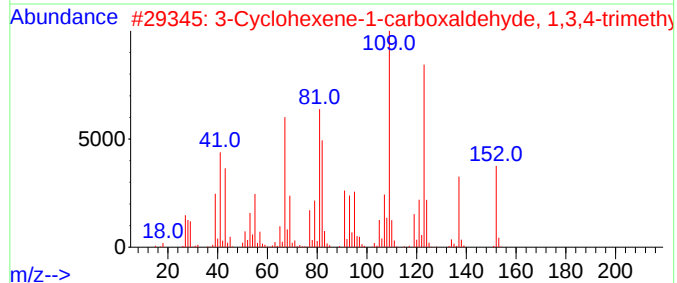
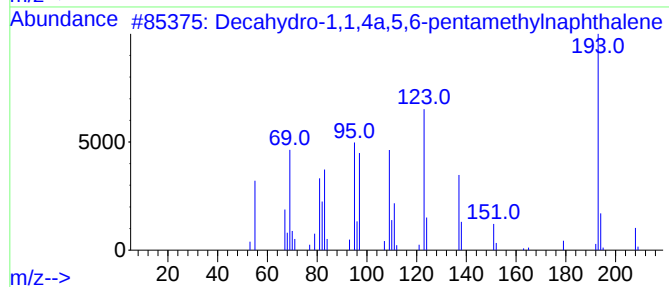
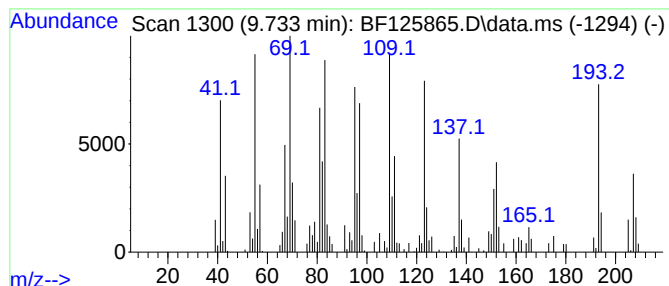
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Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.733	2.63 ng	207971	Acenaphthene-d10	9.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	50
2	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	30
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	27
4	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	25
5	4-Triethylsilylbut-1-en-3-yne	166	C10H18Si	001693-70-5	25



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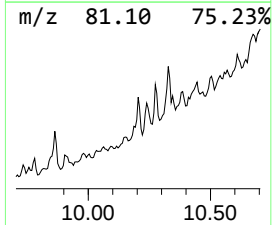
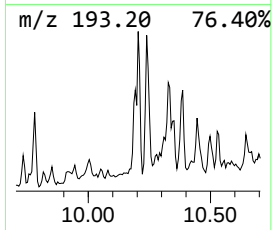
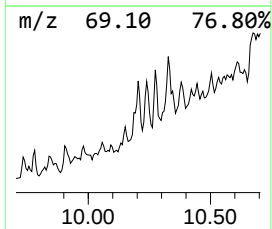
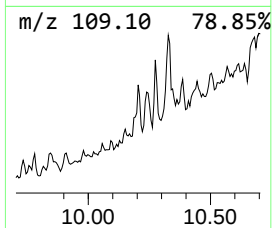
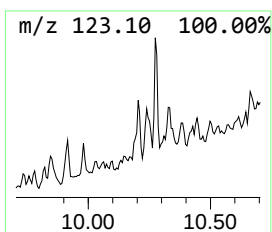
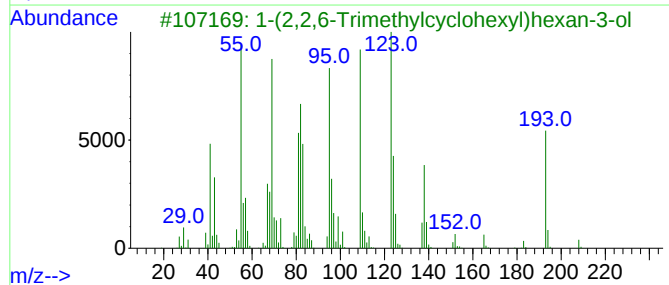
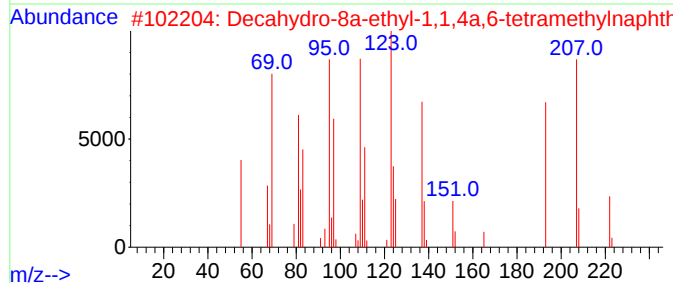
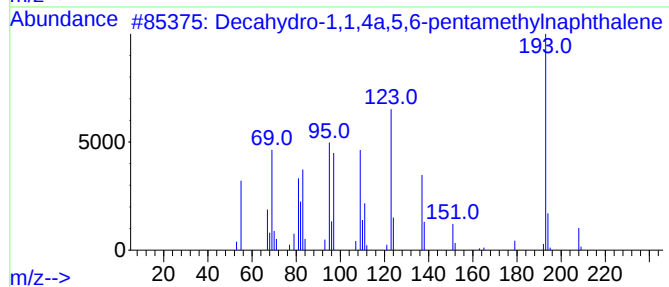
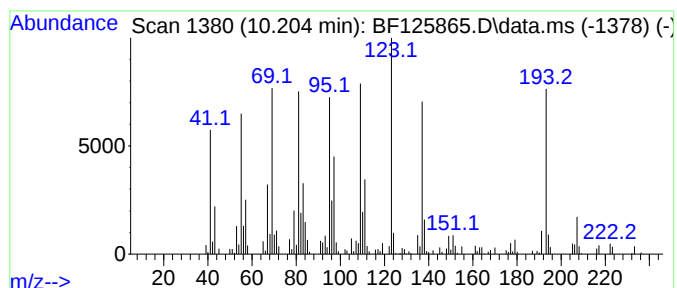
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Peak Number 5 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.204	3.21 ng	254258	Acenaphthene-d10	9.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	78
2	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	68
3	1-(2,2,6-Trimethylcyclohexyl)hex...	226	C15H30O	070788-30-6	47
4	photocitral A	152	C10H16O	055253-28-6	22
5	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	20



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ClientSampleId :
T2-COMP-(1-4)

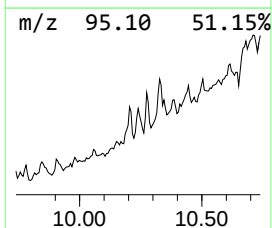
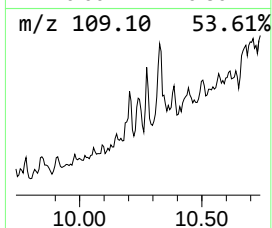
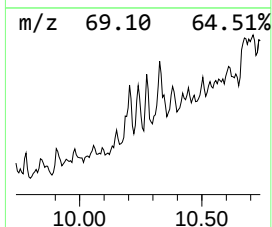
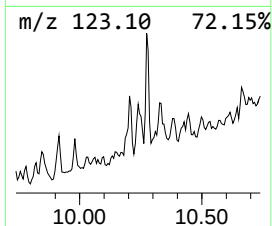
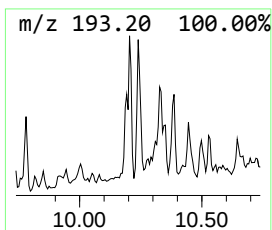
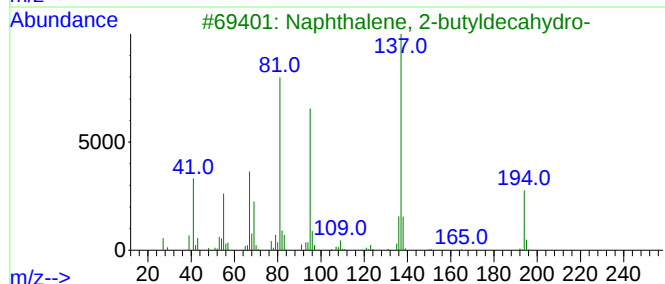
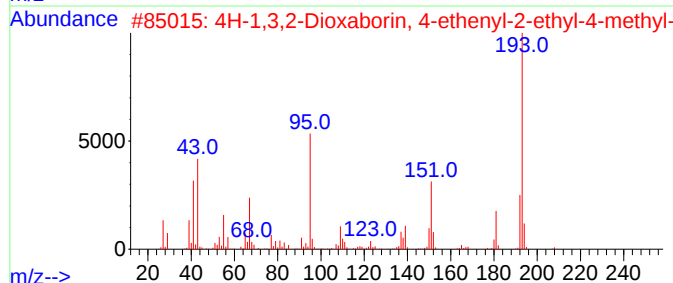
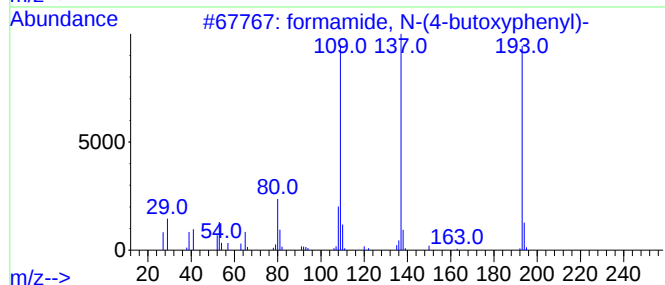
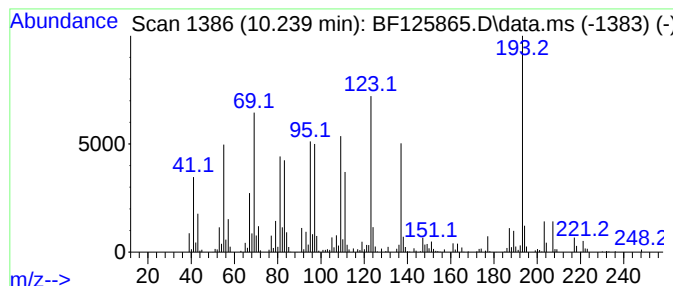
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.239 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.239	5.15 ng	407606	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			formamide, N-(4-butoxyphenyl)-	193	C11H15NO2	1000400-28-0	46
2			4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	38
3			Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	25
4			(2E)-2-Heptylidencyclohexanone	194	C13H22O	173975-69-4	25
5			Cyclopentaneethanol, .beta.,2,3-...	156	C10H20O	021721-18-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125865.D
Acq On : 15 Oct 2021 16:26
Operator : JU/CG
Sample : M4242-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

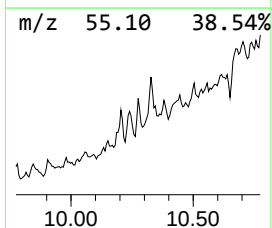
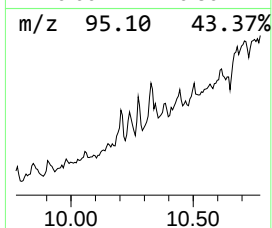
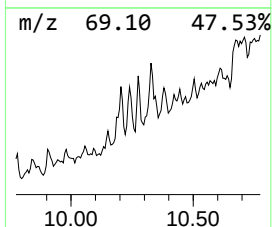
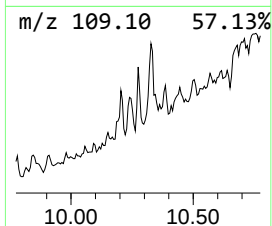
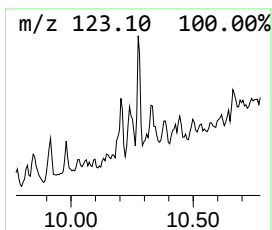
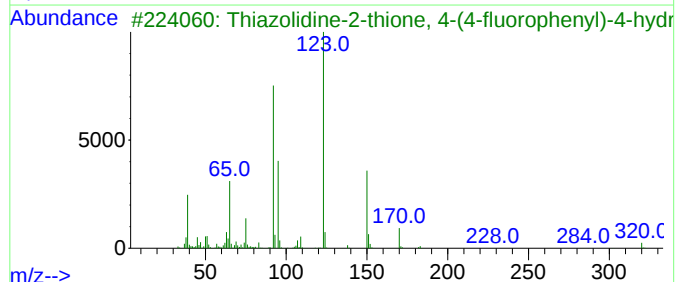
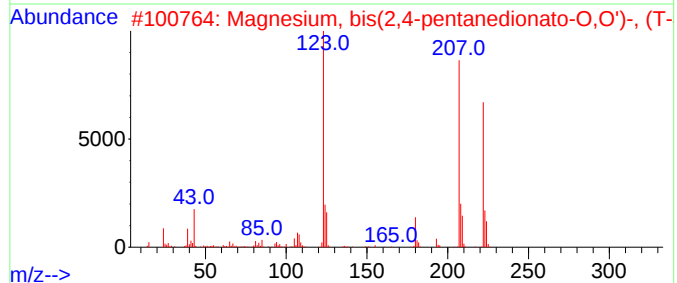
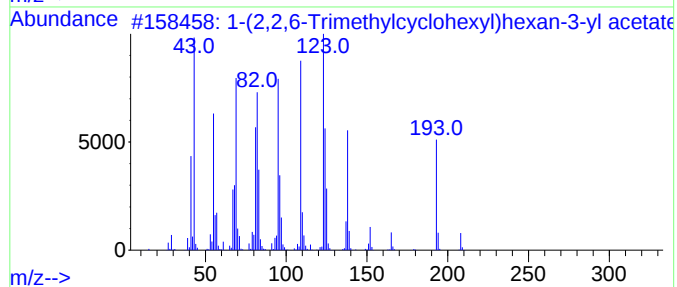
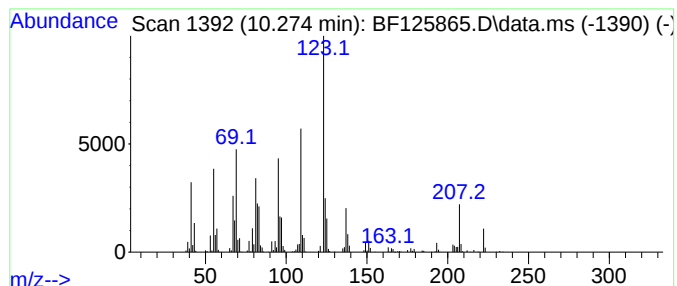
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ClientSampleId :
T2-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-(2,2,6-Trimethylcyclohexy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.275	3.68 ng	291242	Acenaphthene-d10			9.863
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-(2,2,6-Trimethylcyclohexyl)hex...		268	C17H32O2	1000498-96-1	50
2	Magnesium, bis(2,4-pentanedionat...		222	C10H14MgO4	014024-56-7	43
3	Thiazolidine-2-thione, 4-(4-fluo...		320	C15H13FN2O5	1000264-97-7	38
4	1-(1-Ethyl-2,3-dimethyl-cyclopen...		166	C11H18O	1000185-18-6	30
5	Ethanone, 1-[3-[2-methyl-2-(5-me...		222	C13H18O3	080114-28-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125865.D
Acq On : 15 Oct 2021 16:26
Operator : JU/CG
Sample : M4242-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T2-COMP-(1-4)

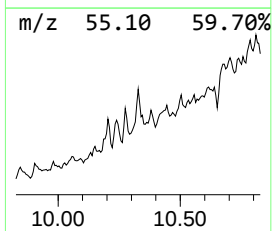
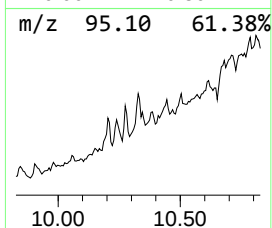
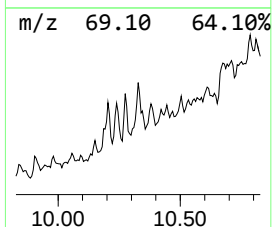
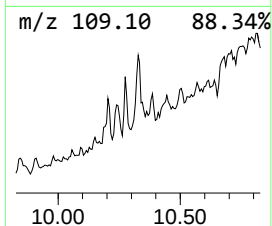
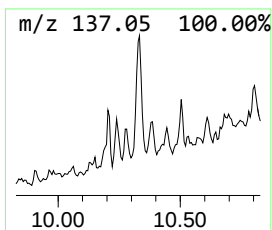
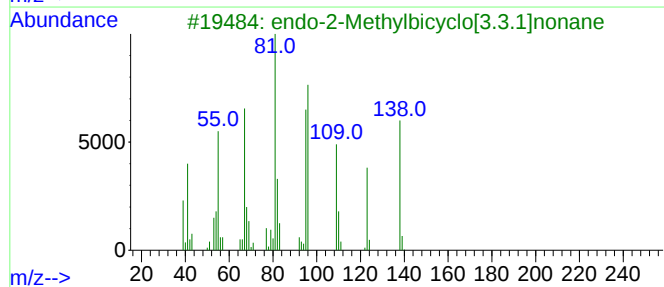
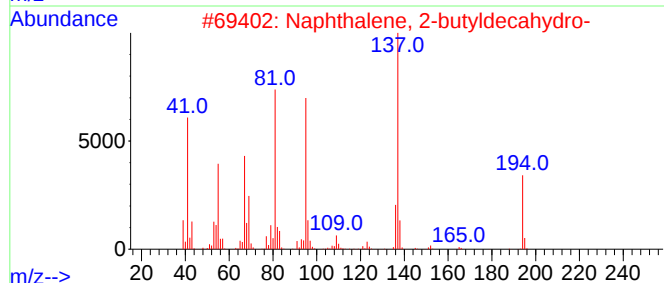
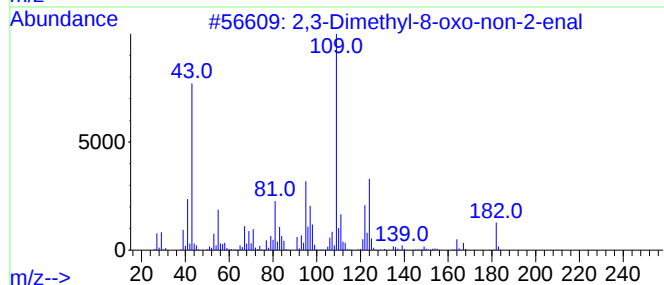
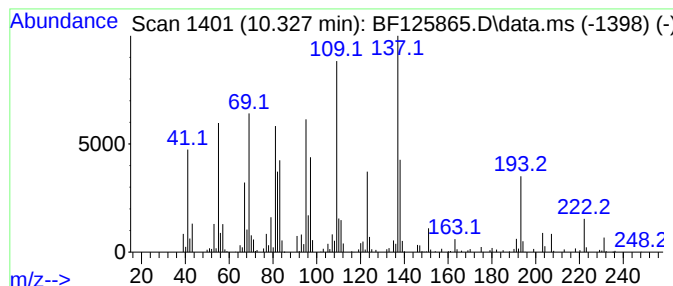
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.327 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.327	6.53 ng	516906	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Dimethyl-8-oxo-non-2-enal	182	C11H18O2	1000186-82-6	38
2			Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	30
3			endo-2-Methylbicyclo[3.3.1]nonane	138	C10H18	042558-37-2	30
4			4-Fluorophenyl isocyanate	137	C7H4FNO	001195-45-5	27
5			1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125865.D
Acq On : 15 Oct 2021 16:26
Operator : JU/CG
Sample : M4242-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T2-COMP-(1-4)

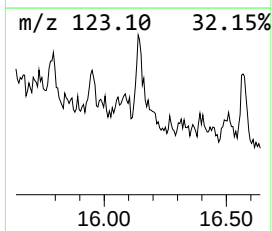
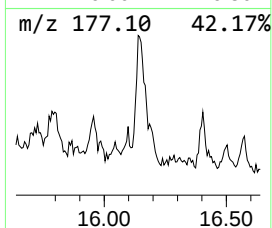
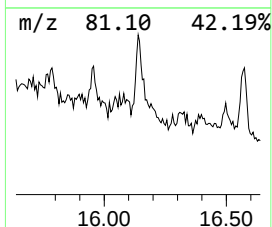
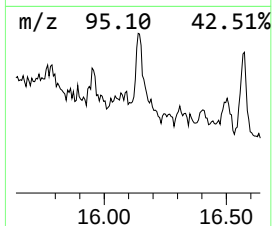
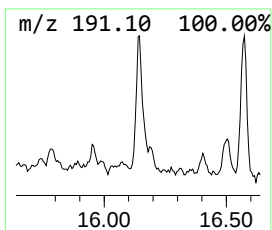
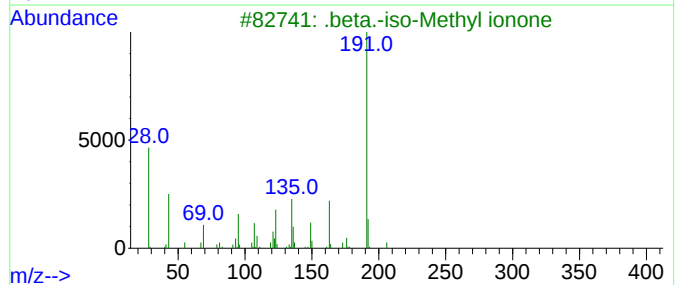
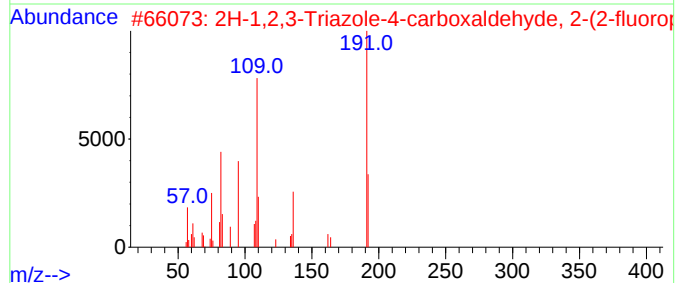
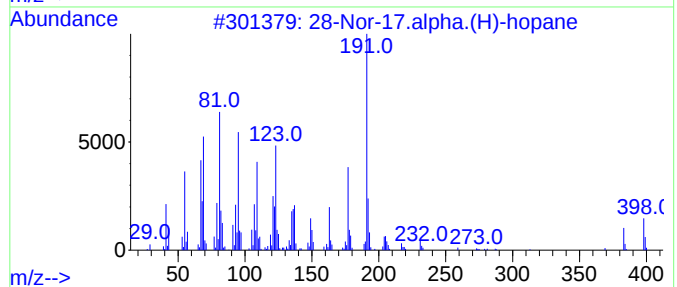
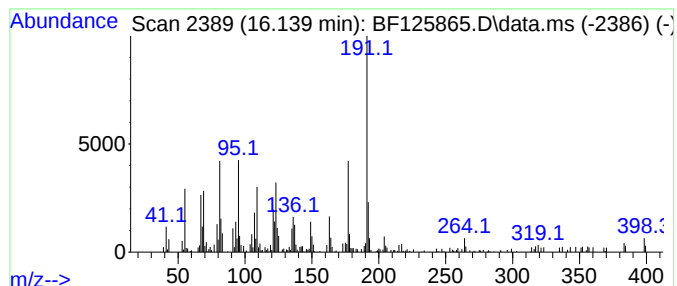
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 28-Nor-17.alpha.(H)-hopane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	8.08 ng	438994	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	89
2			2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	43
3			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
4			17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	41
5			5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125865.D
Acq On : 15 Oct 2021 16:26
Operator : JU/CG
Sample : M4242-21
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T2-COMP-(1-4)

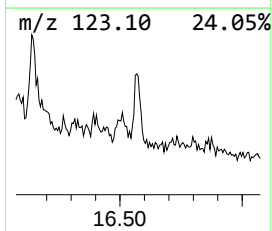
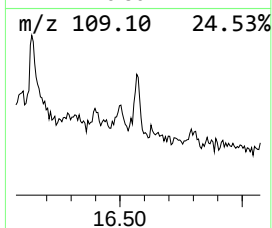
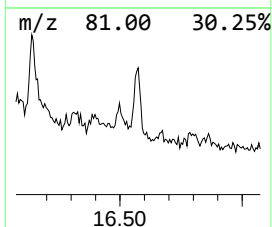
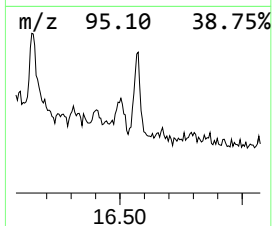
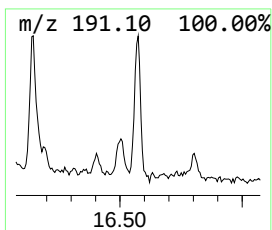
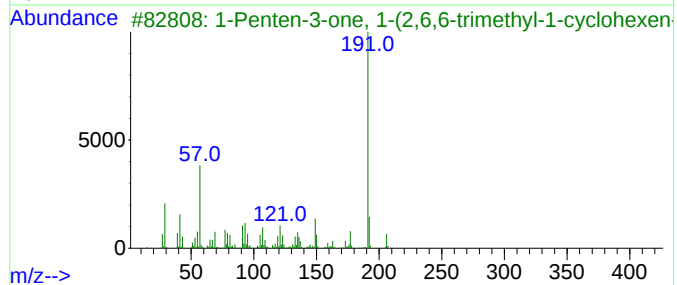
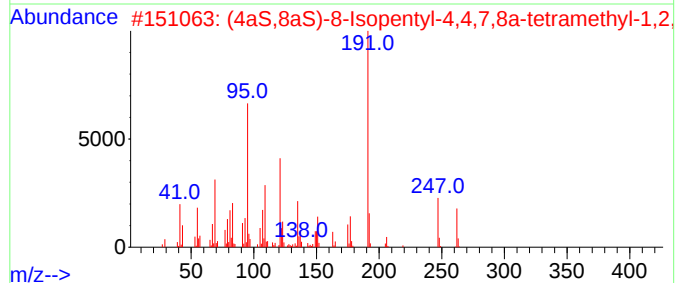
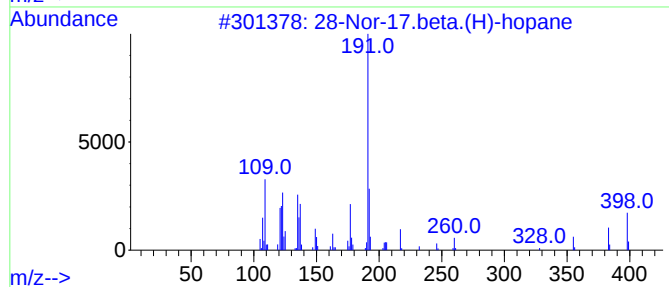
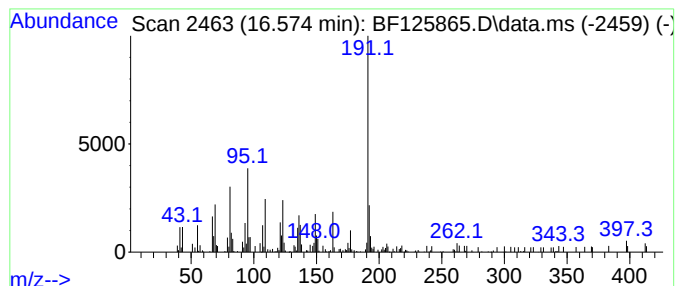
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 28-Nor-17.beta.(H)-hopane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.574	4.14 ng	224971	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	64
2			(4aS,8aS)-8-Isopentyl-4,4,7,8a-t...	262	C19H34	220766-79-0	64
3			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	55
4			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	52
5			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
 Data File : BF125865.D
 Acq On : 15 Oct 2021 16:26
 Operator : JU/CG
 Sample : M4242-21
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T2-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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...	2.122	36.8	ng	1895590	1	6.833	1031650	20.0
unknown5.063	5.063	2.2	ng	111248	1	6.833	1031650	20.0
Ethanol, 2-(2-b...	8.016	3.2	ng	222443	2	8.116	1401770	20.0
Decahydro-1,1,4...	9.733	2.6	ng	207971	3	9.863	1582060	20.0
Decahydro-8a-et...	10.204	3.2	ng	254258	3	9.863	1582060	20.0
unknown10.239	10.239	5.2	ng	407606	3	9.863	1582060	20.0
1-(2,2,6-Trimet...	10.275	3.7	ng	291242	3	9.863	1582060	20.0
unknown10.327	10.327	6.5	ng	516906	3	9.863	1582060	20.0
28-Nor-17.alpha...	16.139	8.1	ng	438994	6	15.439	1086520	20.0
28-Nor-17.beta....	16.574	4.1	ng	224971	6	15.439	1086520	20.0