

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
 Data File : BF126104.D
 Acq On : 10 Nov 2021 13:16
 Operator : JU/CG
 Sample : M4540-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	4	11	17	rBV	1828203	2282475	45.68%	6.426%
2	2.969	144	150	159	rBV2	36414	58223	1.17%	0.164%
3	5.075	504	508	518	rVB	87100	105768	2.12%	0.298%
4	5.475	571	576	579	rBV	4018439	3682406	73.70%	10.367%
5	6.481	742	747	750	rBV	3844928	3781997	75.70%	10.647%
6	6.851	807	810	814	rBV	1122634	921240	18.44%	2.594%
7	7.416	901	906	909	rBV	2612563	2373124	47.50%	6.681%
8	8.039	1008	1012	1024	rBV	342251	389048	7.79%	1.095%
9	8.134	1024	1028	1032	rBV	1309617	1084601	21.71%	3.053%
10	9.210	1206	1211	1214	rBV	5169143	4103667	82.13%	11.553%
11	9.516	1260	1263	1266	rBV2	131191	117669	2.36%	0.331%
12	9.551	1266	1269	1273	rVB	126238	99819	2.00%	0.281%
13	9.804	1308	1312	1314	rBV	140255	120935	2.42%	0.340%
14	9.863	1318	1322	1324	rBV	1069316	897263	17.96%	2.526%
15	9.886	1324	1326	1333	rVB	1359927	1167728	23.37%	3.287%
16	10.010	1344	1347	1350	rVB	246518	185000	3.70%	0.521%
17	10.051	1350	1354	1359	rBV2	107157	101624	2.03%	0.286%
18	10.675	1455	1460	1464	rBV	2581999	2234019	44.71%	6.289%
19	10.710	1464	1466	1471	rVB2	58251	58210	1.17%	0.164%
20	10.869	1490	1493	1502	rVB3	54395	71226	1.43%	0.201%
21	11.375	1575	1579	1582	rBV	1053337	978433	19.58%	2.755%
22	12.957	1844	1848	1851	rBV	3929626	3147856	63.00%	8.862%
23	13.169	1881	1884	1886	rBV	113413	109005	2.18%	0.307%
24	13.610	1956	1959	1962	rBV	83362	78874	1.58%	0.222%
25	13.727	1974	1979	1982	rBV	5889598	4996291	100.00%	14.066%
26	13.863	1998	2002	2011	rBV	252801	343806	6.88%	0.968%
27	14.010	2023	2027	2030	rBV	1098691	911625	18.25%	2.566%
28	14.504	2106	2111	2114	rBV3	80532	136011	2.72%	0.383%
29	14.939	2182	2185	2189	rVB3	68573	68470	1.37%	0.193%
30	15.174	2222	2225	2230	rVB6	48361	61928	1.24%	0.174%
31	15.474	2272	2276	2280	rBV	619329	754576	15.10%	2.124%
32	15.951	2354	2357	2362	rVB2	77994	97513	1.95%	0.275%

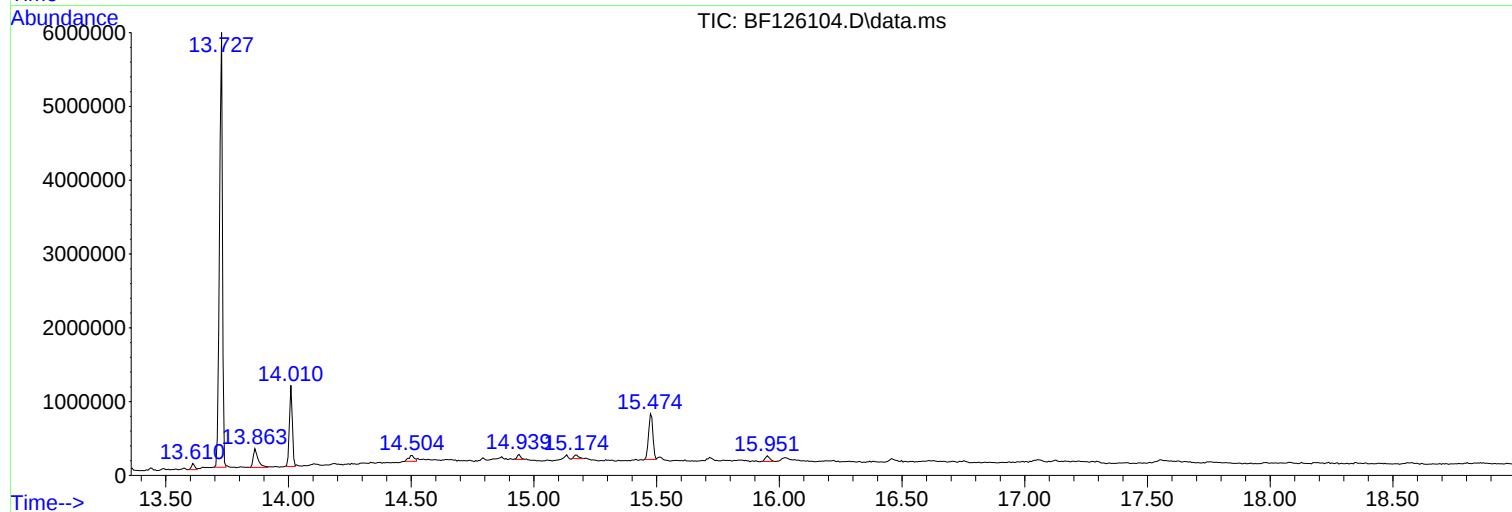
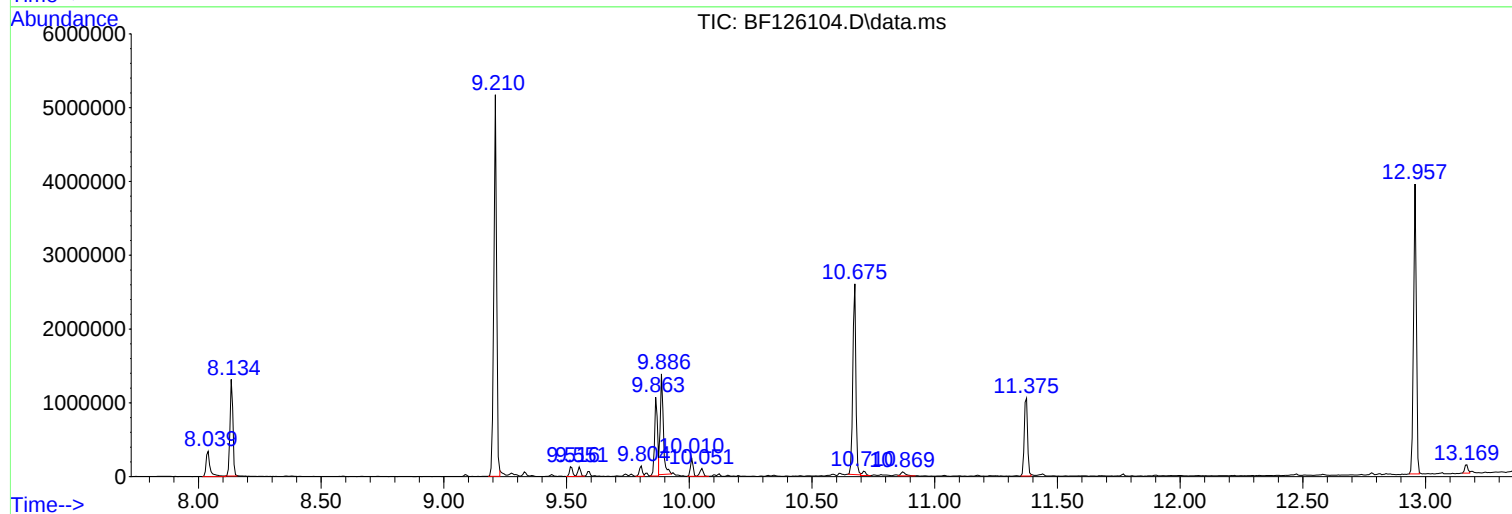
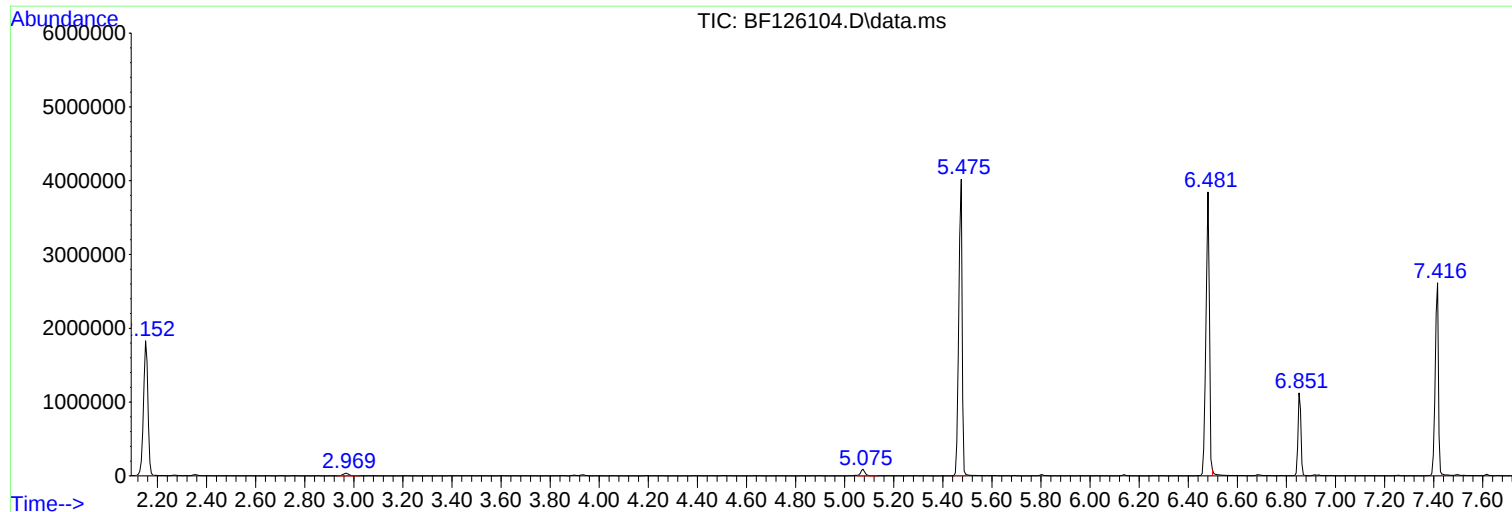
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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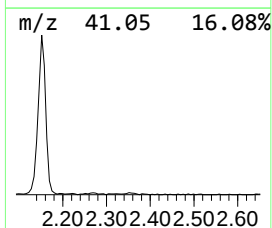
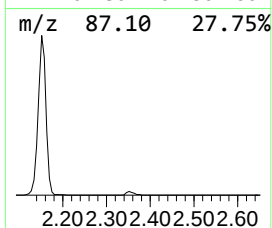
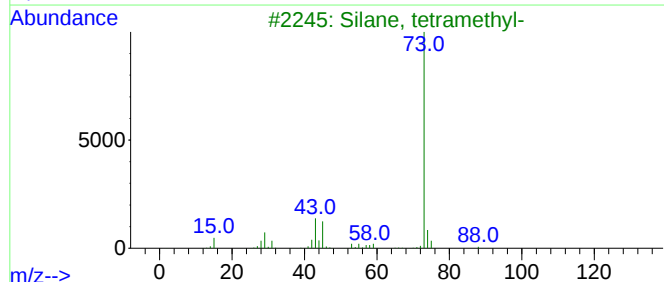
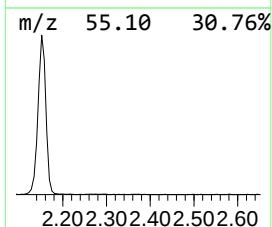
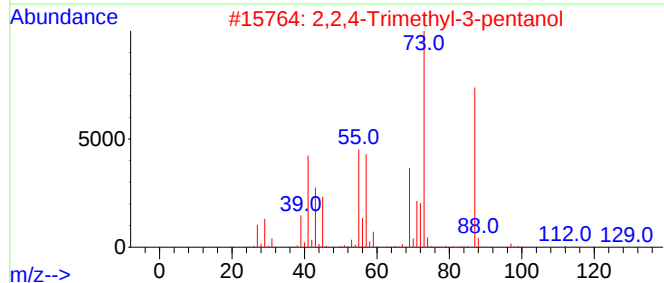
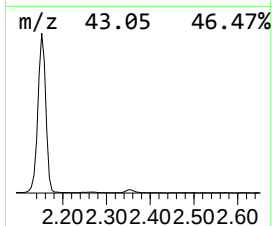
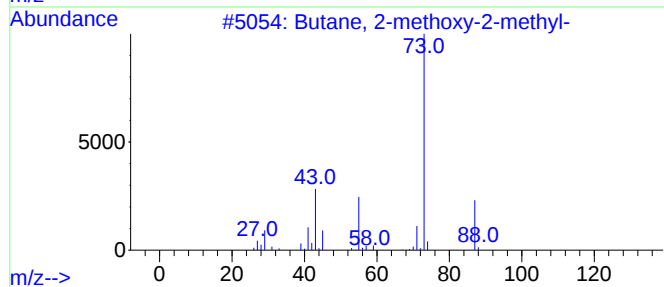
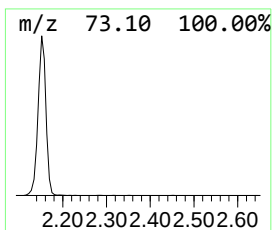
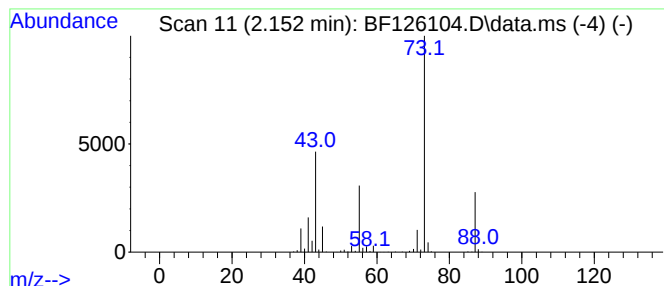
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	49.55 ng	2282480	1,4-Dichlorobenzene-d4	6.851

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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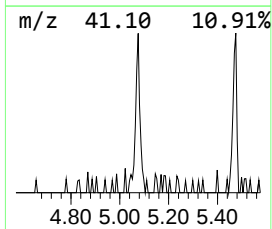
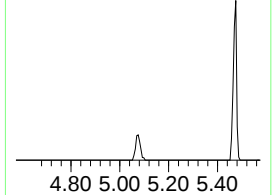
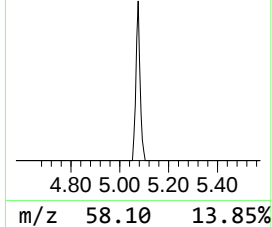
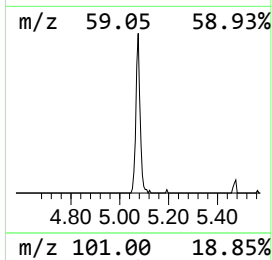
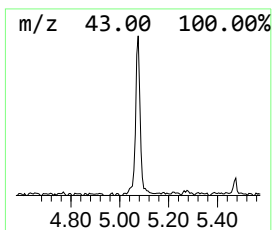
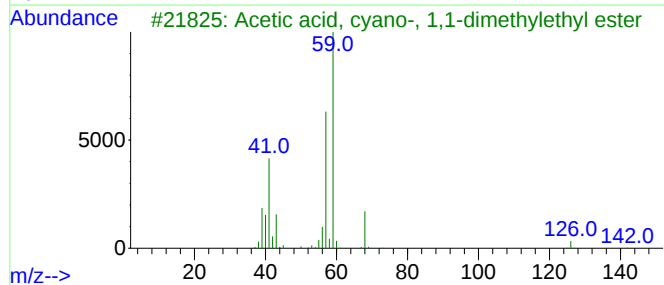
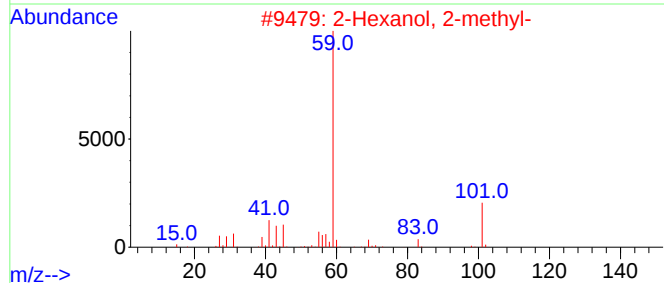
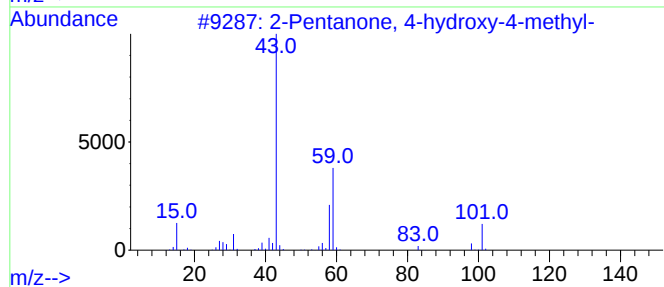
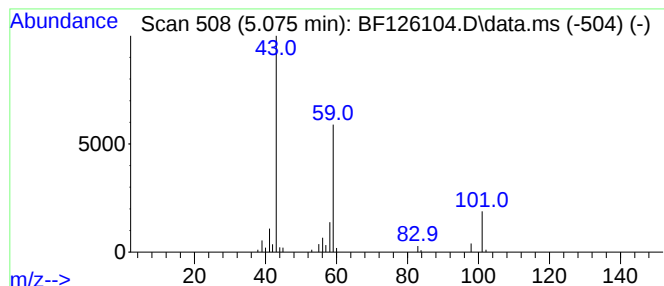
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	2.30 ng	105768	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4			3-Octanol	130	C8H18O	000589-98-0	33
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28



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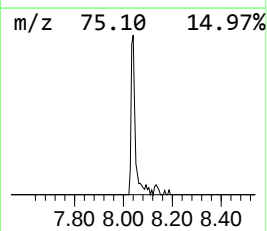
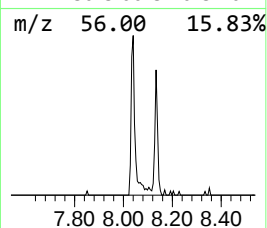
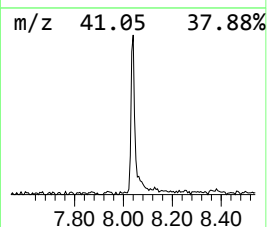
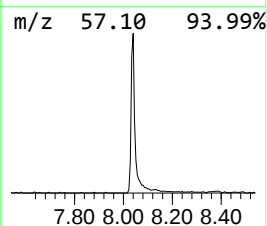
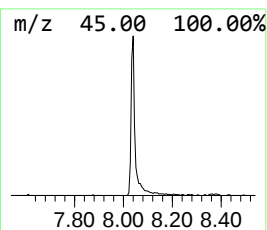
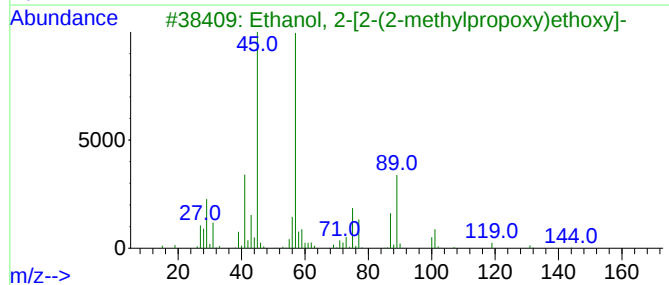
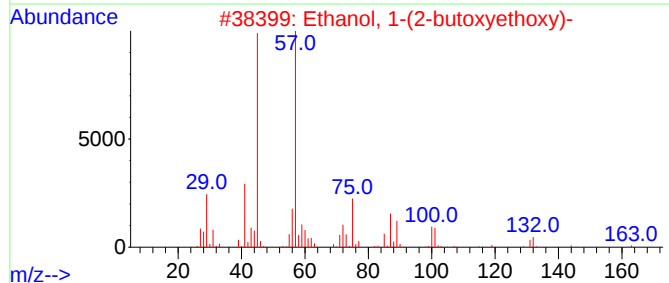
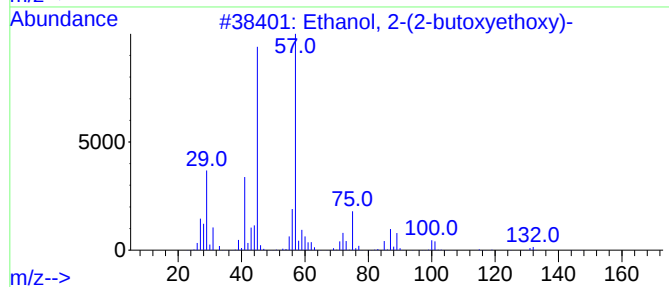
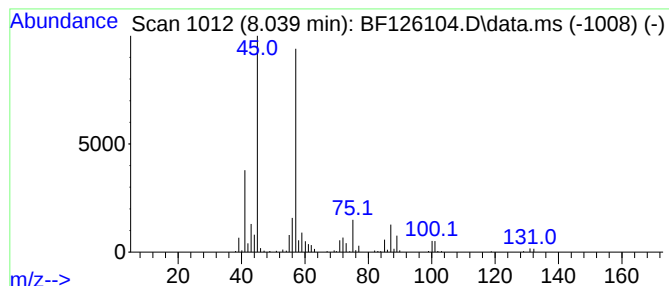
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	7.17 ng	389048	Naphthalene-d8	8.134

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	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	53



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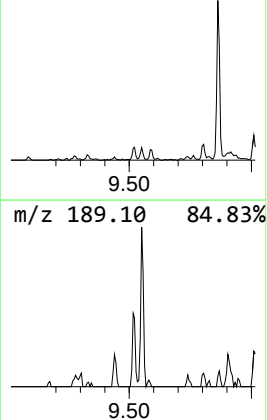
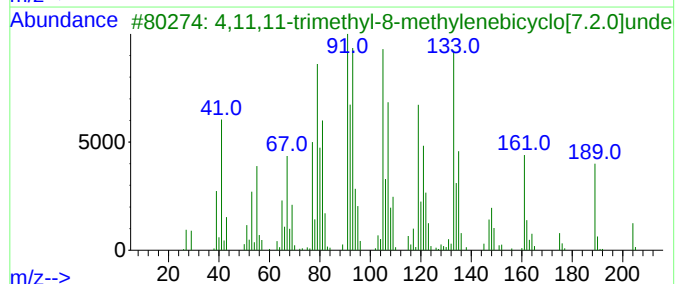
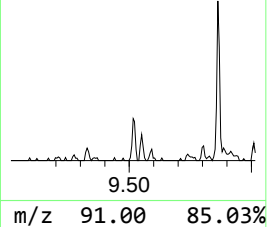
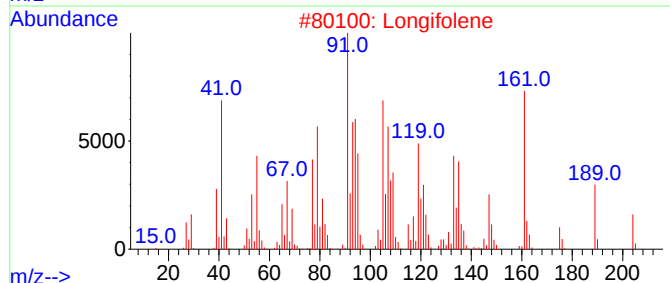
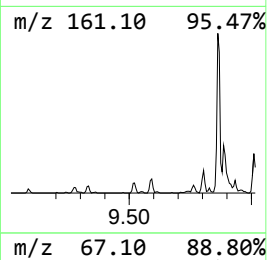
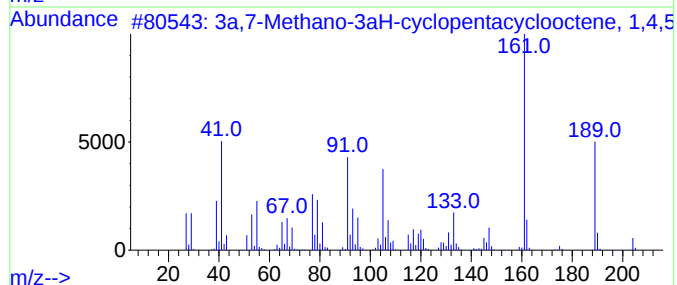
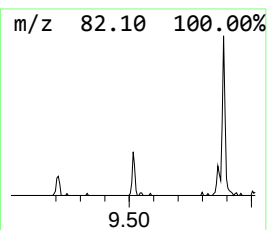
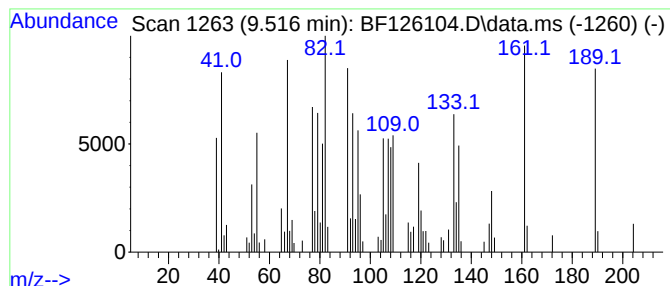
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3a,7-Methano-3aH-cyclopenta... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.516	2.02 ng	117669	Acenaphthene-d10	9.886	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3a,7-Methano-3aH-cyclopentacyclo...	204	C15H24	000469-92-1	72
2	Longifolene	204	C15H24	000475-20-7	64
3	4,11,11-trimethyl-8-methylenebic...	204	C15H24	889360-49-0	51
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	44
5	6-(4-Fluorophenyl)-2-hydroxypyri...	189	C11H8FNO	1010509-20-5	30



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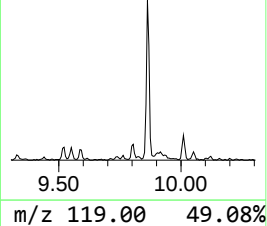
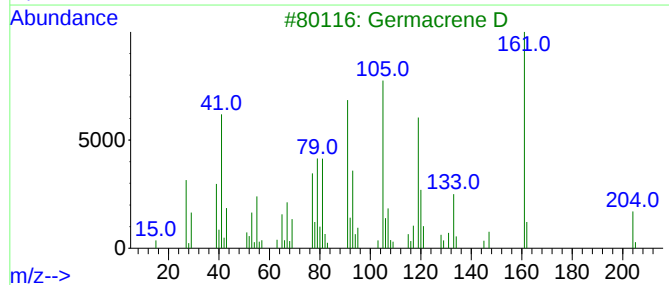
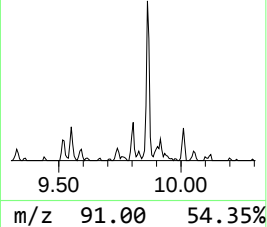
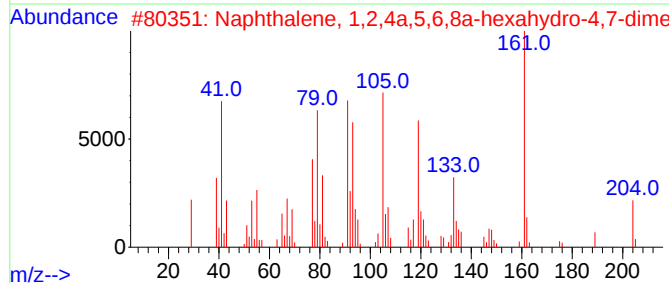
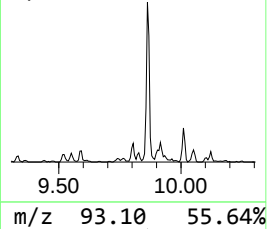
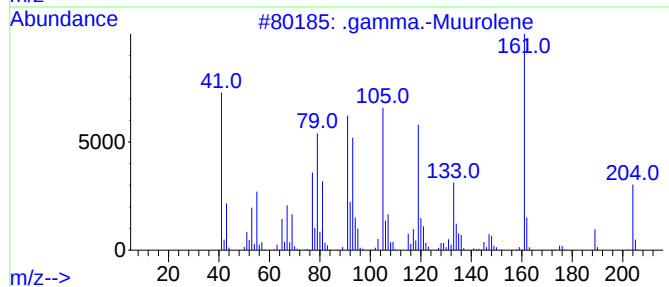
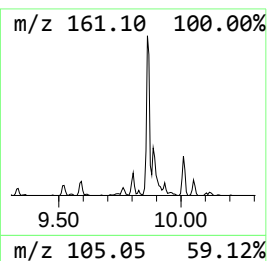
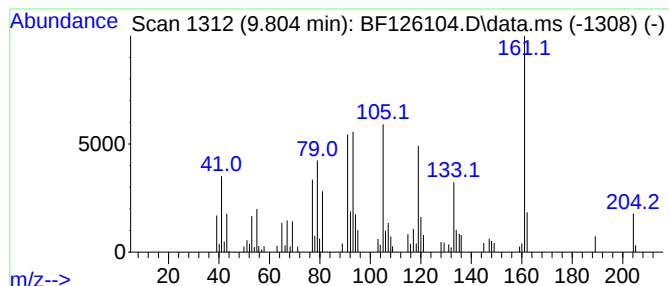
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 .gamma.-Muurolene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	2.07 ng	120935	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Muurolene	204	C15H24	030021-74-0	97
2			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	96
3			Germacrene D	204	C15H24	023986-74-5	94
4			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	89
5			1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	86



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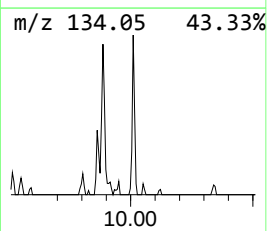
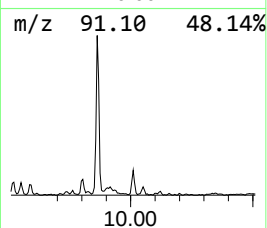
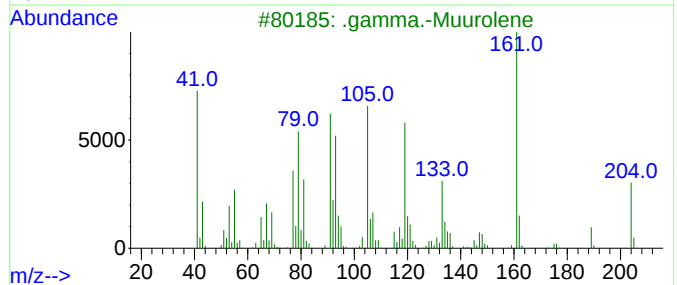
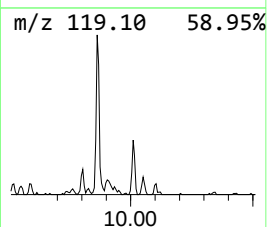
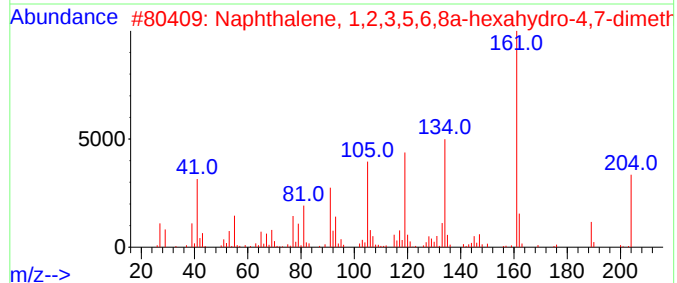
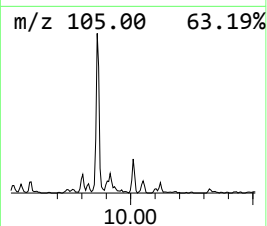
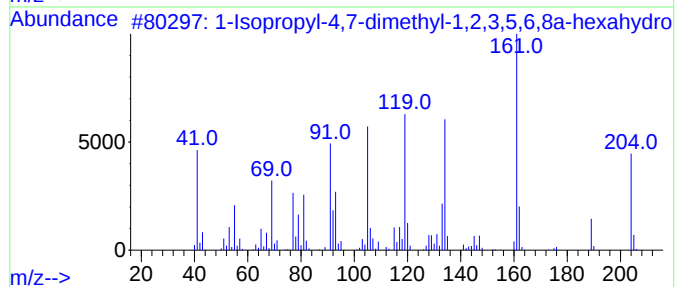
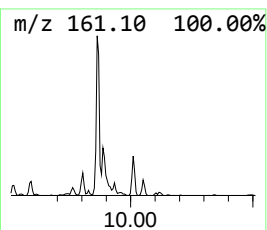
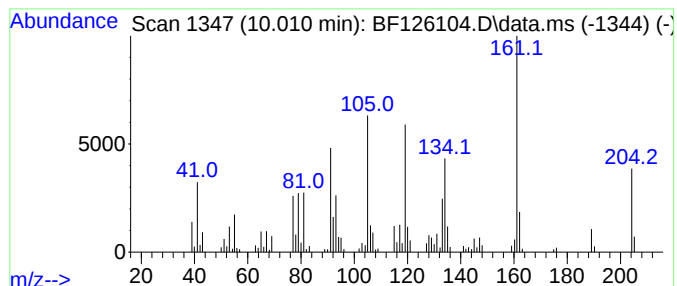
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Isopropyl-4,7-dimethyl-1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	3.17 ng	185000	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	99
2			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	97
3			.gamma.-Murolene	204	C15H24	030021-74-0	93
4			(1S,4aR,8aS)-1-Isopropyl-7-methy...	204	C15H24	006980-46-7	89
5			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126104.D
Acq On : 10 Nov 2021 13:16
Operator : JU/CG
Sample : M4540-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

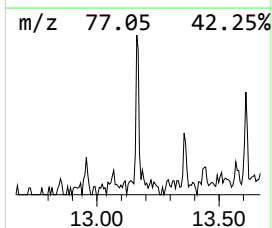
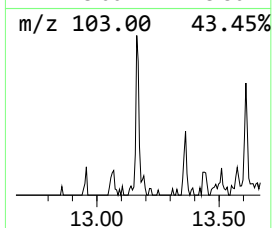
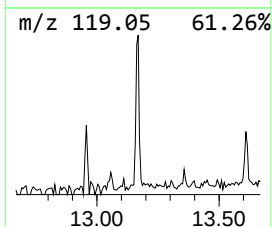
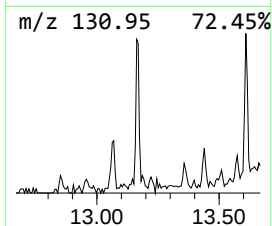
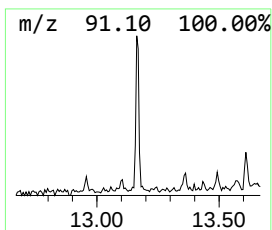
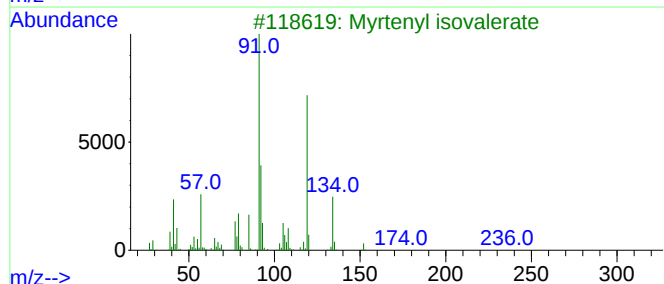
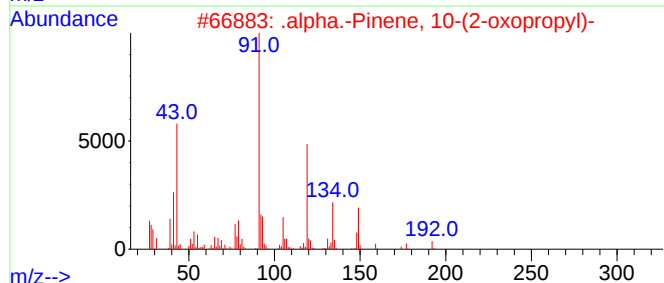
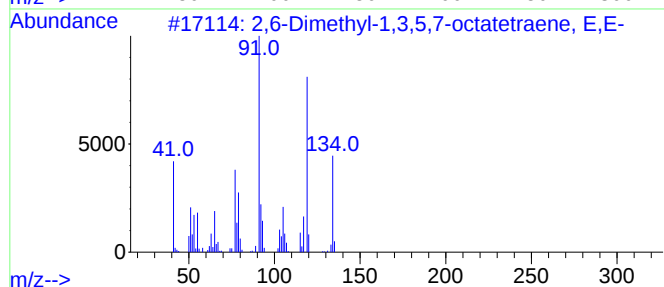
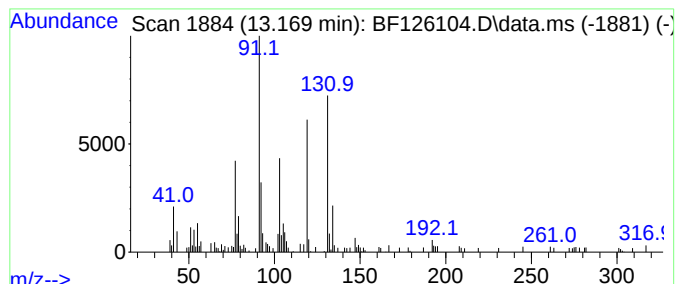
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,6-Dimethyl-1,3,5,7-octate... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.169	2.39 ng	109005	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-1,3,5,7-octatetraen...	134	C10H14	000460-01-5	58
2	.alpha.-Pinene, 10-(2-oxopropyl)-	192	C13H20O	1010159-36-3	45
3	Myrtenyl isovalerate	236	C15H24O2	033900-84-4	38
4	Myrtenyl angelate	234	C15H22O2	138530-45-7	38
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126104.D
Acq On : 10 Nov 2021 13:16
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Sample : M4540-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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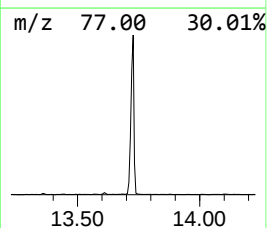
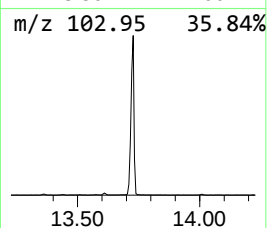
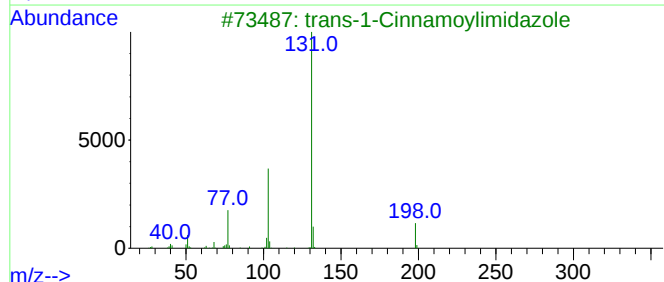
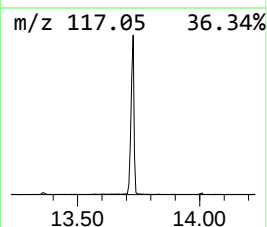
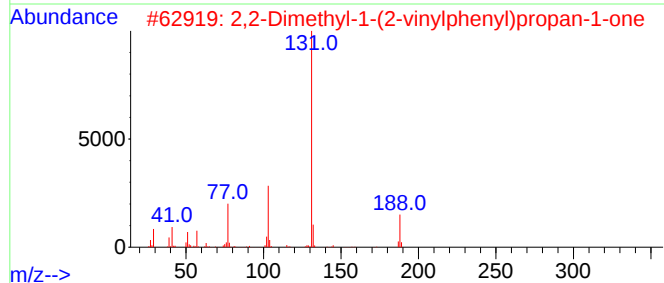
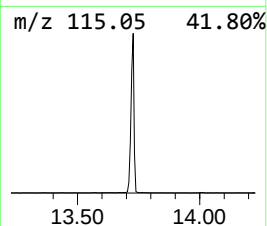
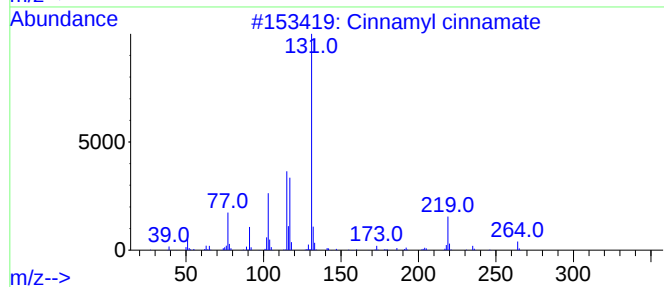
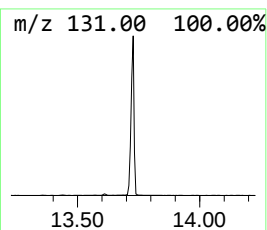
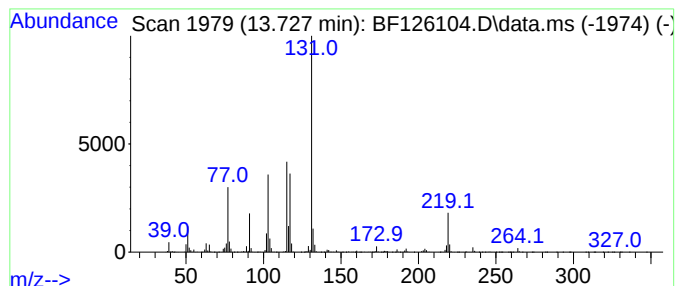
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	109.61 ng	4996290	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	60
3			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
4			Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	47
5			1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126104.D
Acq On : 10 Nov 2021 13:16
Operator : JU/CG
Sample : M4540-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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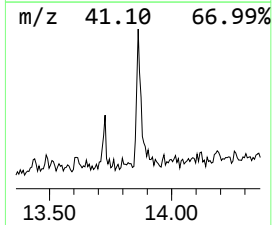
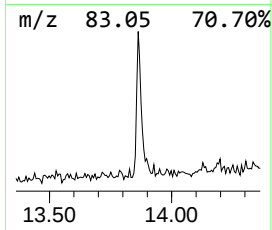
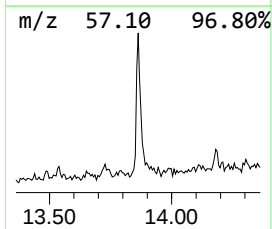
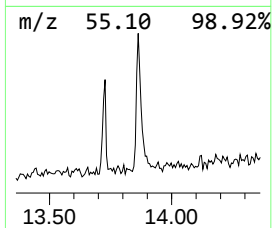
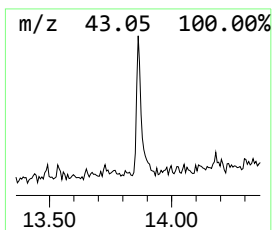
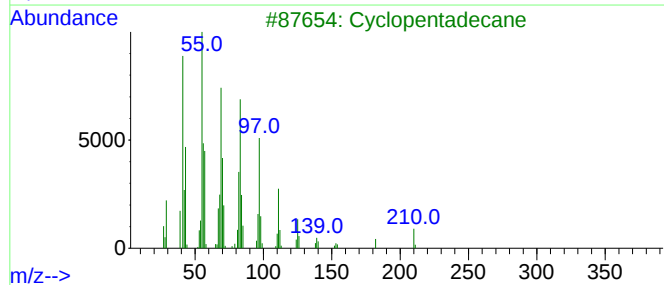
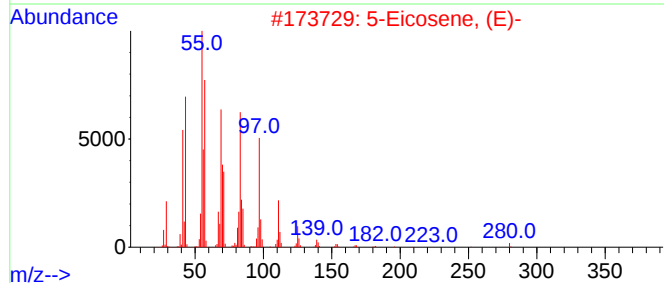
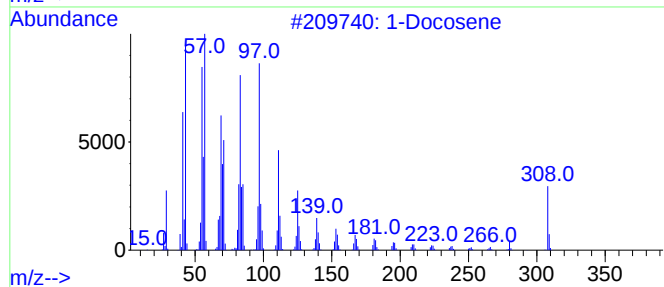
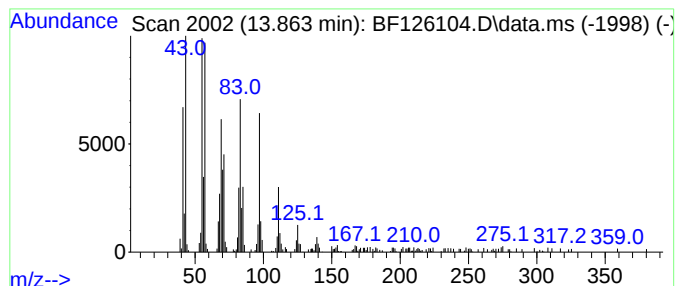
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	7.54 ng	343806	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	5-Eicosene, (E)-			280	C20H40	074685-30-6	94
3	Cyclopentadecane			210	C15H30	000295-48-7	94
4	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
5	Cyclotetracosane			336	C24H48	000297-03-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126104.D
Acq On : 10 Nov 2021 13:16
Operator : JU/CG
Sample : M4540-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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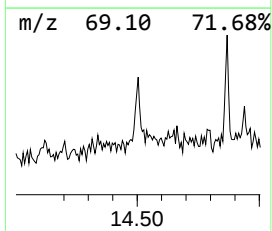
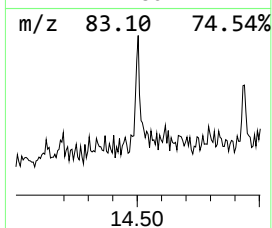
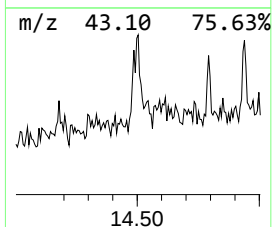
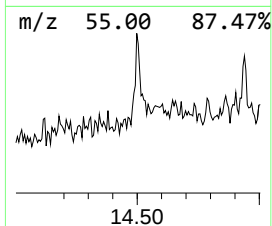
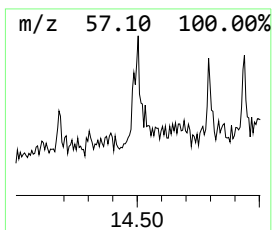
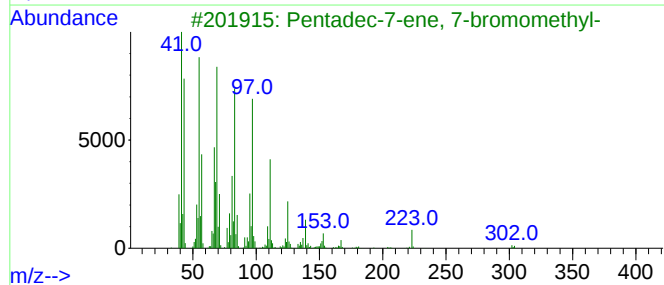
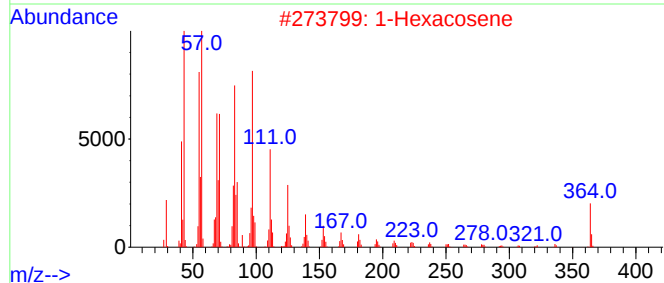
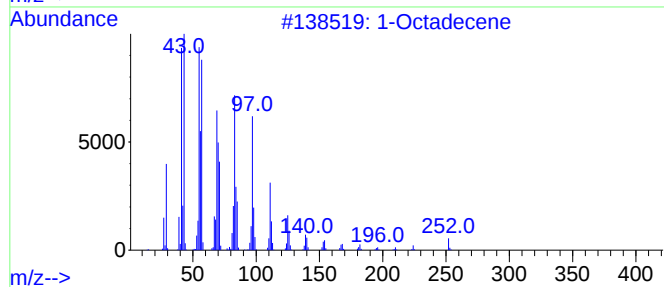
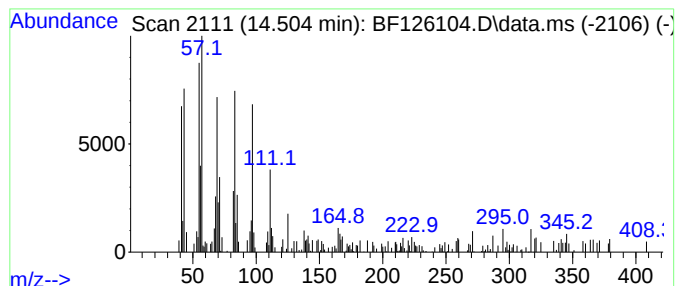
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	2.98 ng	136011	Chrysene-d12	14.010

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecene	252	C18H36	000112-88-9	90
2		1-Hexacosene	364	C26H52	018835-33-1	90
3		Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	89
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
5		Heptacos-1-ene	378	C27H54	015306-27-1	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126104.D
Acq On : 10 Nov 2021 13:16
Operator : JU/CG
Sample : M4540-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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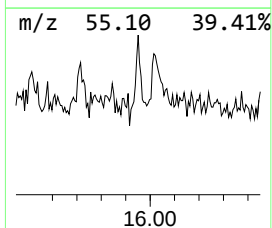
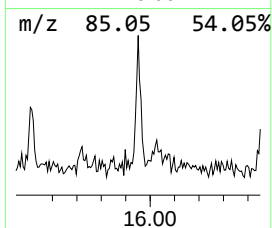
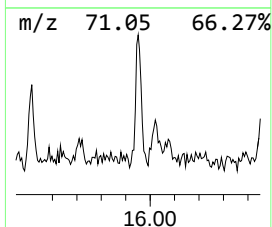
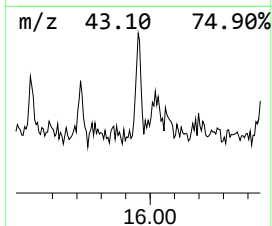
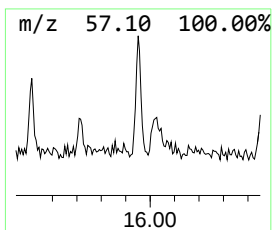
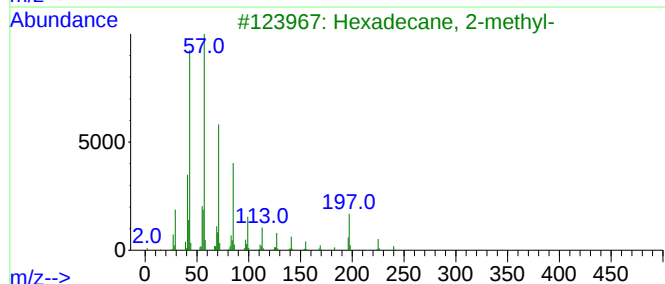
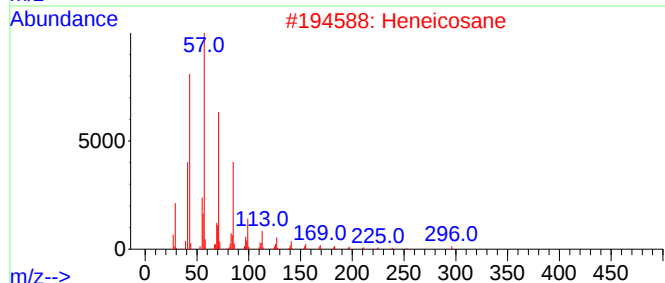
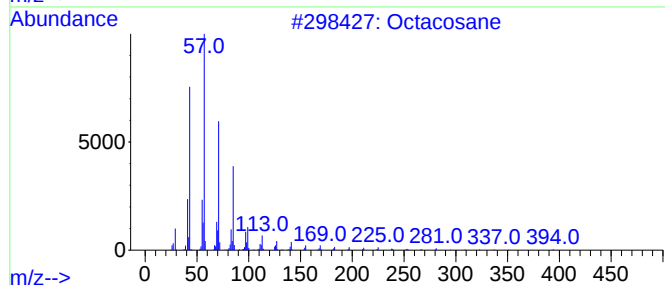
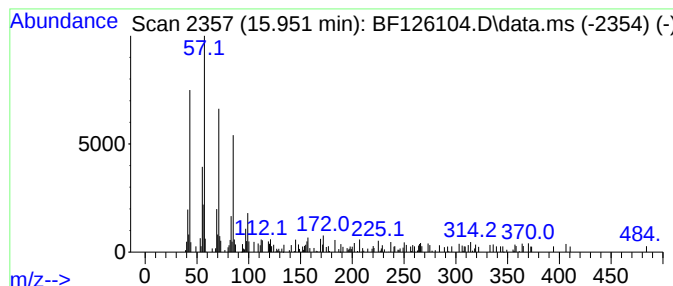
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.58 ng	97513	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	86
2			Heneicosane	296	C21H44	000629-94-7	62
3			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	62
4			Tridecane, 2-methyl-	198	C14H30	001560-96-9	62
5			Nonadecane	268	C19H40	000629-92-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126104.D
Acq On : 10 Nov 2021 13:16
Operator : JU/CG
Sample : M4540-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
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2-Pentanone, 4-...	5.075	2.3	ng	105768	1	6.851	921240	20.0
Ethanol, 2-(2-b...	8.039	7.2	ng	389048	2	8.134	1084600	20.0
3a,7-Methano-3a...	9.516	2.0	ng	117669	3	9.886	1167730	20.0
.gamma.-Murolene	9.804	2.1	ng	120935	3	9.886	1167730	20.0
1-Isopropyl-4,7...	10.010	3.2	ng	185000	3	9.886	1167730	20.0
2,6-Dimethyl-1,...	13.169	2.4	ng	109005	5	14.010	911625	20.0
Cinnamyl cinnamate	13.727	109.6	ng	4996290	5	14.010	911625	20.0
1-Docosene	13.863	7.5	ng	343806	5	14.010	911625	20.0
1-Octadecene	14.504	3.0	ng	136011	5	14.010	911625	20.0
Octacosane	15.951	2.6	ng	97513	6	15.474	754576	20.0